

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 JAN 02 STN pricing information for 2008 now available
NEWS 3 JAN 16 CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 4 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 5 JAN 28 MARPAT searching enhanced
NEWS 6 JAN 28 USGENE now provides USPTO sequence data within 3 days of publication
NEWS 7 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 8 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements
NEWS 9 FEB 08 STN Express, Version 8.3, now available
NEWS 10 FEB 20 PCI now available as a replacement to DPCI
NEWS 11 FEB 25 IFIREF reloaded with enhancements
NEWS 12 FEB 25 IMSPRODUCT reloaded with enhancements
NEWS 13 FEB 29 WPIINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS 14 MAR 31 IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS 15 MAR 31 CAS REGISTRY enhanced with additional experimental spectra
NEWS 16 MAR 31 CA/Caplus and CASREACT patent number format for U.S. applications updated
NEWS 17 MAR 31 LPCI now available as a replacement to LDPCI
NEWS 18 MAR 31 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 19 APR 04 STN AnaVist, Version 1, to be discontinued
NEWS 20 APR 15 WPIDS, WPIINDEX, and WPIX enhanced with new predefined hit display formats
NEWS 21 APR 28 EMBASE Controlled Term thesaurus enhanced
NEWS 22 APR 28 IMSRESEARCH reloaded with enhancements
NEWS 23 MAY 30 INPAFAMDB now available on STN for patent family searching
NEWS 24 MAY 30 DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS 25 JUN 06 EPFULL enhanced with 260,000 English abstracts
NEWS 26 JUN 06 KOREAPAT updated with 41,000 documents
NEWS 27 JUN 13 USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 06:11:32 ON 16 JUN 2008

```
=> e reg1
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
The EXPAND command is used to look at the index in a file
which has an index. This file does not have an index.
```

=> file reg
COST IN U.S. DOLLARS
SINCE FILE ENTRY TOTAL
SESSION
0.21 0.21
FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 06:11:49 ON 16 JUN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES: 15 JUN 2008 HIGHEST RN 1028329-25-0
DICTIONARY FILE UPDATES: 15 JUN 2008 HIGHEST RN 1028329-25-0

New CAS Information Use Policies - enter HELP USAGETERMS for details

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stndgen/stndoc/properties.html>

=> logoff hold
COST IN U.S. DOLLARS

| | SINCE FILE ENTRY | TOTAL SESSION |
|---------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.46 | 0.67 |

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 06:12:14 ON 16 JUN 2008

Connecting via Winsock to STM

Welcome to STN International! Enter x::x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 06:33:40 ON 16 JUN 2008
FILE 'REGISTRY' ENTERED AT 06:33:40 ON 16 JUN 2008
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| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.46 | 0.67 |

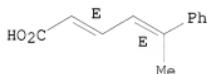
=> e 2,4-Hexadienoic acid, 5-phenyl-, (E,E)-/cn
E1 1 2,4-HEXADIENOIC ACID, 5-NITRO-, METHYL ESTER, (E,E)-/CN
E2 1 2,4-HEXADIENOIC ACID, 5-NITRO-8-QUINOLINYL ESTER/CN
E3 1 --> 2,4-HEXADIENOIC ACID, 5-PHENYL-, (E,E)-/CN
E4 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, (Z,E)-/CN
E5 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, BUTYL ESTER, (2E,4E)-/CN
E6 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, ETHYL ESTER, (E,Z)-/CN
E7 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER/CN
E8 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (2E,4E)-/CN
E9 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (E,?)-/CN
E10 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (E,E)-/CN
E11 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (Z,?)-/CN
E12 1 2,4-HEXADIENOIC ACID, 6,6,6-TRICHLORO-/CN

=> e3
L1 1 "2,4-HEXADIENOIC ACID, 5-PHENYL-, (E,E)-"/CN

=> d 11

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 28028-84-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2,4-Hexadienoic acid, 5-phenyl-, (E,E)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Sorbic acid, 5-phenyl-, (E,E)- (8CI)
FS STEREOSEARCH
MF C12 H12 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 8.53 | 8.74 |

FILE 'CAPLUS' ENTERED AT 06:34:56 ON 16 JUN 2008
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FILE COVERS 1907 - 16 Jun 2008 VOL 148 ISS 25
FILE LAST UPDATED: 15 Jun 2008 (20080615/ED)

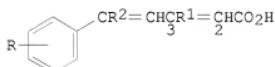
Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> ll
L2 2 L1

=> d 12 1-2 ti fbib abs

L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
TI Structure-antitranspirant activity relation in a series of abscisic acid
analogues
AN 1992:2232 CAPLUS
DN 116:2232
OREF 116:459a,462a
TI Structure-antitranspirant activity relation in a series of abscisic acid
analogues
AU Dimoglo, A. S.; Ustyugov, V. A.; Popa, D. P.; Kuchkova, K. I.
CS Inst. Khim., Kishinev, USSR
SO Buletinul Academiei de Stiinte a Republicii Moldova, Stiinte Biologice si
Chimice (1991), (1), 49-55
CODEN: IAMNEN; ISSN: 1019-5289
DT Journal
LA Russian
GI



I

AB Consideration of electronic-topological matrixes of 46 I (R = e.g., H, Cl, Me, or OMe, R¹ and R² = H or Me; 2,3-E or Z) demonstrated that the surface of the triangle formed by neg. charged atoms, the perimeter/surface ratio, and the ratio of the total charge of these atoms to the triangle surface determine the antitranspirant activity of I in barley. Linear positioning of the 3 neg. charged moieties, the absence of the neg. center in the aromatic ring, and the absence of Me at the pentadienoic acid radical made I

inactive. A cis-trans isomerization interaction with the positioning of the moiety in the aromatic ring was essential for activity. Me at C₄ was best positioned for the activity. Steric factors also affected activity. The effectiveness of these criteria for the selection of antitranspirants is illustrated using the known antitranspirant vomifoliol.

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
 TI Influence of the substituent and the geometry of the double bond on dissociation constants of cinnamylideneacetic acids
 AN 1970:110633 CAPLUS
 DN 72:110633
 OREF 72:19963a,19966a
 TI Influence of the substituent and the geometry of the double bond on dissociation constants of cinnamylideneacetic acids
 AU Molho, Darius; Giraud, Michel
 CS Lab. Chim., Museum Nat. Hist. Natur., Paris, Fr.
 SO Bulletin de la Societe Chimique de France (1969), (12), 4447-52
 CODEN: BSCFAS; ISSN: 0037-8968
 DT Journal
 LA French
 GI For diagram(s), see printed CA Issue.
 AB trans,trans-Cinnamylideneacetic acids I are more acidic than acids II. The acidity of ring substituted acids follows a Hammett relation. β-Methylcinnamylideneacetic acids are less acidic than the δ-methyl acids. Steric factors have very little effect.

| | | | |
|--|------------|---------|--|
| => file reg | | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL | |
| FULL ESTIMATED COST | ENTRY | SESSION | |
| | 14.94 | 23.68 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL | |
| CA SUBSCRIBER PRICE | ENTRY | SESSION | |
| | -1.60 | -1.60 | |

FILE 'REGISTRY' ENTERED AT 06:46:22 ON 16 JUN 2008
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STRUCTURE FILE UPDATES: 15 JUN 2008 HIGHEST RN 1028329-25-0
 DICTIONARY FILE UPDATES: 15 JUN 2008 HIGHEST RN 1028329-25-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e el

E1 1 2, 4-HEXADIENOIC ACID, 5-METHYL-6-OXO-, METHYL ESTER, (Z,E)-/CN
 E2 1 2, 4-HEXADIENOIC ACID, 5-NITRO-, METHYL ESTER/CN
 E3 1 --> 2, 4-HEXADIENOIC ACID, 5-NITRO-, METHYL ESTER, (E,E)-/CN
 E4 1 2, 4-HEXADIENOIC ACID, 5-NITRO-8-QUINOLINYL ESTER/CN
 E5 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (E,E)-/CN
 E6 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (Z,E)-/CN
 E7 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, BUTYL ESTER, (2E,4E)-/CN
 E8 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, ETHYL ESTER, (E,Z)-/CN
 E9 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER/CN
 E10 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (2E,4E)-/CN
 E11 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (E,?)-/CN
 E12 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (E,E)-/CN

=> e el

E1 1 2, 4-HEXADIENOIC ACID, 5-METHYL-6-OXO-, METHYL ESTER, (2E,4E)-/CN
 E2 1 2, 4-HEXADIENOIC ACID, 5-METHYL-6-OXO-, METHYL ESTER, (E,E)-/CN
 E3 1 --> 2, 4-HEXADIENOIC ACID, 5-METHYL-6-OXO-, METHYL ESTER, (Z,E)-/CN
 E4 1 2, 4-HEXADIENOIC ACID, 5-NITRO-, METHYL ESTER/CN
 E5 1 2, 4-HEXADIENOIC ACID, 5-NITRO-, METHYL ESTER, (E,E)-/CN
 E6 1 2, 4-HEXADIENOIC ACID, 5-NITRO-8-QUINOLINYL ESTER/CN
 E7 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (E,E)-/CN
 E8 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (Z,E)-/CN
 E9 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, BUTYL ESTER, (2E,4E)-/CN
 E10 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, ETHYL ESTER, (E,Z)-/CN
 E11 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER/CN
 E12 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (2E,4E)-/CN

=> e el

E1 1 2, 4-HEXADIENOIC ACID, 5-METHYL-6-OXO-, ETHYL ESTER, (E,E)-/CN
 E2 1 2, 4-HEXADIENOIC ACID, 5-METHYL-6-OXO-, ETHYL ESTER, (Z,E)-/CN
 E3 1 --> 2, 4-HEXADIENOIC ACID, 5-METHYL-6-OXO-, METHYL ESTER, (2E,4E)-/CN
 E4 1 2, 4-HEXADIENOIC ACID, 5-METHYL-6-OXO-, METHYL ESTER, (E,E)-/CN
 E5 1 2, 4-HEXADIENOIC ACID, 5-METHYL-6-OXO-, METHYL ESTER, (Z,E)-/CN
 E6 1 2, 4-HEXADIENOIC ACID, 5-NITRO-, METHYL ESTER/CN
 E7 1 2, 4-HEXADIENOIC ACID, 5-NITRO-, METHYL ESTER, (E,E)-/CN
 E8 1 2, 4-HEXADIENOIC ACID, 5-NITRO-8-QUINOLINYL ESTER/CN
 E9 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (E,E)-/CN
 E10 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (Z,E)-/CN
 E11 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, BUTYL ESTER, (2E,4E)-/CN
 E12 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, ETHYL ESTER, (E,Z)-/CN

=> 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (E,E)-

MISSING OPERATOR '-PHENYL-, (E,E'

=> e 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (E,E)-/CN/cn

E1 1 2, 4-HEXADIENOIC ACID, 5-NITRO-8-QUINOLINYL ESTER/CN
 E2 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (E,E)-/CN
 E3 0 --> 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (E,E)-/CN/CN
 E4 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, (Z,E)-/CN
 E5 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, BUTYL ESTER, (2E,4E)-/CN
 E6 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, ETHYL ESTER, (E,Z)-/CN
 E7 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER/CN
 E8 1 2, 4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (2E,4E)-/CN

E9 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (E,?) - /CN
 E10 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (E,E) - /CN
 E11 1 2,4-HEXADIENOIC ACID, 5-PHENYL-, METHYL ESTER, (Z,?) - /CN
 E12 1 2,4-HEXADIENOIC ACID, 6,6,6-TRICHLORO- /CN

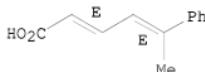
=> e2

L3 1 "2,4-HEXADIENOIC ACID, 5-PHENYL-, (E,E)-" /CN

=> d 13

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 28028-84-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2,4-Hexadienoic acid, 5-phenyl-, (E,E)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Sorbic acid, 5-phenyl-, (E,E)- (8CI)
FS STEREORESEARCH
MF C12 H12 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```

=> logoff hold
COST IN U.S. DOLLARS                               SINCE FILE      TOTAL
                                                    ENTRY        SESSION
FULL ESTIMATED COST                           12.67        36.35

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                    ENTRY        SESSION
CA SUBSCRIBER PRICE                            0.00        -1.60

```

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 06:53:45 ON 16 JUN 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | |
|------|----|--|
| NEWS | 1 | Web Page for STN Seminar Schedule - N. America |
| NEWS | 2 | JAN 02 |
| NEWS | 3 | JAN 16 |
| | | CAS patent coverage enhanced to include exemplified prophetic substances |
| NEWS | 4 | JAN 28 |
| | | USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats |
| NEWS | 5 | JAN 28 |
| | | MARPAT searching enhanced |
| NEWS | 6 | JAN 28 |
| | | USGENE now provides USPTO sequence data within 3 days of publication |
| NEWS | 7 | JAN 28 |
| NEWS | 8 | JAN 28 |
| | | TOXCENTER enhanced with reloaded MEDLINE segment MEDLINE and LMEDLINE reloaded with enhancements |
| NEWS | 9 | FEB 08 |
| | | STN Express, Version 8.3, now available |
| NEWS | 10 | FEB 20 |
| | | PCI now available as a replacement to DPCI |
| NEWS | 11 | FEB 25 |
| | | IFIREFI reloaded with enhancements |
| NEWS | 12 | FEB 25 |
| | | IMSPRODUCT reloaded with enhancements |
| NEWS | 13 | FEB 29 |
| | | WPINDEX/WPIIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification |
| NEWS | 14 | MAR 31 |
| | | IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats |
| NEWS | 15 | MAR 31 |
| | | CAS REGISTRY enhanced with additional experimental spectra |
| NEWS | 16 | MAR 31 |
| | | CA/Caplus and CASREACT patent number format for U.S. applications updated |
| NEWS | 17 | MAR 31 |
| | | LPCI now available as a replacement to LDPCI |
| NEWS | 18 | MAR 31 |
| | | EMBASE, EMBAL, and LEMBASE reloaded with enhancements |
| NEWS | 19 | APR 04 |
| | | STN AnaVist, Version 1, to be discontinued |
| NEWS | 20 | APR 15 |
| | | WPIIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats |
| NEWS | 21 | APR 28 |
| | | EMBASE Controlled Term thesaurus enhanced |
| NEWS | 22 | APR 28 |
| | | IMSRESEARCH reloaded with enhancements |
| NEWS | 23 | MAY 30 |
| | | INPAFAMDB now available on STN for patent family searching |
| NEWS | 24 | MAY 30 |
| | | DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option |
| NEWS | 25 | JUN 06 |
| | | EPFULL enhanced with 260,000 English abstracts |
| NEWS | 26 | JUN 06 |
| | | KOREPAT updated with 41,000 documents |
| NEWS | 27 | JUN 13 |
| | | USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications |

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 14:51:35 ON 18 JUN 2008

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL

FULL ESTIMATED COST

ENTRY SESSION
0.42 0.42

FILE 'REGISTRY' ENTERED AT 14:52:25 ON 18 JUN 2008
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STRUCTURE FILE UPDATES: 17 JUN 2008 HIGHEST RN 1028750-52-8
DICTIONARY FILE UPDATES: 17 JUN 2008 HIGHEST RN 1028750-52-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

```
=> e dehydrolipoic acid/cn
E1          1      DEHYDROLINALYL FORMATE/CN
E2          1      DEHYDROLINDESTRENOLIDE/CN
E3          0 --> DEHYDROLIPOIC ACID/CN
E4          1      DEHYDROLIRINIDINE/CN
E5          1      DEHYDROLIRIOFERINE/CN
E6          1      DEHYDROLIRIOFERINE ACETATE/CN
E7          1      DEHYDROLITHOCHOLIC ACID/CN
E8          1      DEHYDROLOBINALINE/CN
E9          1      DEHYDROLOGANIN/CN
E10         1      DEHYDROLOLIOLID/E/CN
E11         1      DEHYDROLONGILOBOL/CN
E12         1      DEHYDROLONGISTROBINE/CN

=> e lipoic acid/cn
E1          1      LIPOHYDROPEROXIDASE/CN
E2          1      LIPOIC ACETYLTRANSFERASE/CN
E3          2 --> LIPOIC ACID/CN
E4          1      LIPOIC ACID ACETYLTRANSFERASE/CN
E5          1      LIPOIC ACID CHLORIDE/CN
E6          1      LIPOIC ACID DEHYDROGENASE/CN
E7          1      LIPOIC ACID DISULFONE/CN
E8          1      LIPOIC ACID FREE RADICAL/CN
E9          1      LIPOIC ACID METHYL ESTER/CN
E10         1      LIPOIC ACID SYNTHASE/CN
E11         1      LIPOIC ACID SYNTHASE (ARABIDOPSIS THALIANA CLONE PRACE-5'/19
3K14/PBLUE-3' GENE LIP1 PRECURSOR)/CN
E12         1      LIPOIC ACID SYNTHASE (CAULOBACTER CRESCENTUS GENE CC1735)/CN

=> e3
L1          2      "LIPOIC ACID"/CN

=> d 11 1-2
```

L1 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN
RN 57828-26-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Lipoic acid (CA INDEX NAME)
MF Unspecified
CI COM, MAN
LC STN Files: ADISNEWS, AGRICOLA, BIOSIS, CA, CAPLUS, CASREACT, CIN, PROMT,
SCISEARCH, TOXCENTER, USPAT2, USPATFULL

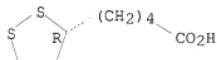
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

684 REFERENCES IN FILE CA (1907 TO DATE)
35 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
684 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1200-22-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,2-Dithiolane-3-pentanoic acid, (3R)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2-Dithiolane-3-pentanoic acid, (R)-
CN 1,2-Dithiolane-3-valeric acid, (+)- (8CI)
OTHER NAMES:
CN (R)-(+)- α -Lipoic acid
CN (R)- α -Lipoic acid
CN (R)-Lipoic acid
CN α -(+)-Lipoic acid
CN α -Lipoic acid
CN Byodinoral 300
CN d-Thioctic acid
CN Lipoec
CN Lipoic acid
CN R-(+)-Thioctic acid
CN Thiogamma
CN Tiobec
CN Tiobec Retard
FS STEREOSEARCH
MF C8 H14 O2 S2
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO,
CA, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN,
CSCHEM, EMBASE, IFICDB, IFIUDB, IMSDRUGNEWS, IMSRESEARCH, IPA, MRCK*,
NAPRALERT, PROMT, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, USPATOLD
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2239 REFERENCES IN FILE CA (1907 TO DATE)
98 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2250 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> e 1,2-Dithiolane-3-pent-3-enoic acid /cn

E1 1 1,2-DITHIOLANE-3-OCTANOIC ACID, 4-(ACETYLAMINO)PHENYL ESTER/CN
CN

E2 1 1,2-DITHIOLANE-3-OCTANOIC ACID, 5-HEPTYL-, METHYL ESTER/CN

E3 0 --> 1,2-DITHIOLANE-3-PENT-3-ENOIC ACID/CN

E4 1 1,2-DITHIOLANE-3-PENTANAL/CN

E5 1 1,2-DITHIOLANE-3-PENTANAMIDE/CN

E6 1 1,2-DITHIOLANE-3-PENTANAMIDE, (±)-, POLYMER WITH 2-PROPEN
ENITRILE/CN

E7 1 1,2-DITHIOLANE-3-PENTANAMIDE, (±)-, POLYMER WITH ETHENYL
ACETATE/CN

E8 1 1,2-DITHIOLANE-3-PENTANAMIDE, (±)-, POLYMER WITH METHYL 2
-PROPENONE/CN

E9 1 1,2-DITHIOLANE-3-PENTANAMIDE, (3R)-/CN

E10 1 1,2-DITHIOLANE-3-PENTANAMIDE, (3S)-/CN

E11 1 1,2-DITHIOLANE-3-PENTANAMIDE, (R)-/CN

E12 1 1,2-DITHIOLANE-3-PENTANAMIDE, (R)-, MIXT. WITH 5-HYDROXY-2-(
HYDROXYMETHYL)-4H-PYRAN-4-ONE/CN

=>
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary
files\10025947\10025947 lipoics.str



chain nodes :
6 7 8 9 10
ring nodes :
1 2 3 4 5
chain bonds :
1-6 6-7 7-8 8-9 9-10
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 6-7 7-8 8-9
exact bonds :
1-6 9-10

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

L2 STRUCTURE UPLOADED

=> d 12
L2 HAS NO ANSWERS
L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 12 sss sam

SAMPLE SEARCH INITIATED 14:59:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 23 TO ITERATE

100.0% PROCESSED 23 ITERATIONS
SEARCH TIME: 00.00.01

13 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 173 TO 747
PROJECTED ANSWERS: 44 TO 476

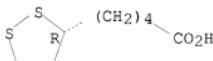
L3 13 SEA SSS SAM L2

=> d scan

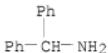
L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,2-Dithiolane-3-pentanoic acid, (R)-, compd. with α -phenylbenzenemethanamine (1:1) (9CI)
MF C13 H13 N . C8 H14 O2 S2

CM 1

Absolute stereochemistry. Rotation (+).



CM 2

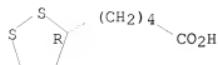


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):13

L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Cystine, (R)-1,2-dithiolane-3-pentanoate (9CI)
MF C8 H14 O2 S2 . x C6 H12 N2 O4 S2

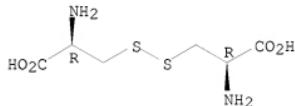
CM 1

Absolute stereochemistry. Rotation (+).



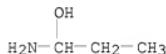
CM 2

Absolute stereochemistry.



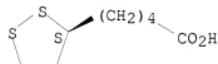
L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,2-Dithiolane-3-pentanoic acid, (3S)-, compd. with l-amino-l-propanol
(1:1) (9CI)
MF C8 H14 O2 S2 . C3 H9 N O

CM 1

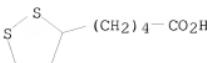


CM 2

Absolute stereochemistry. Rotation (-).



L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,2-Dithiolane-3-pentanoic acid, zinc salt, hydrate (2:1:2)
MF C8 H14 O2 S2 . H2 O . 1/2 Zn

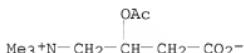


● H₂O

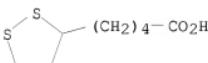
● 1/2 Zn

L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1-Propanaminium, 2-(acetyloxy)-3-carboxy-N,N,N-trimethyl-, inner salt,
mixt. with 1,2-dithiolane-3-pentanoic acid (9CI)
MF C9 H17 N O4 . C8 H14 O2 S2
CI MXS

CM 1

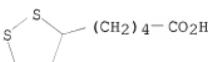


CM 2

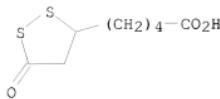


L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,2-Dithiolane-3-valeric acid, dimer, DL- (8CI)
MF (C8 H14 O2 S2)2
CI PMS

CM 1



L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,2-Dithiolane-3-pentanoic acid, 5-oxo-
MF C8 H12 O3 S2



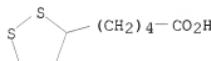
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Vitamin B12, mixt. with 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methylthiazolium chloride, 1,2-dithiolane-3-pentanoic acid, riboflavin and vitamin B6 (9CI)
MF C63 H88 Co N14 O14 P . C17 H20 N4 O6 . C12 H17 N4 O S . C8 H14 O2 S2 . Cl
. Unspecified
CI MXS

CM 1

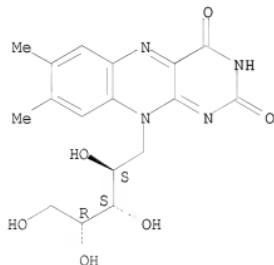
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

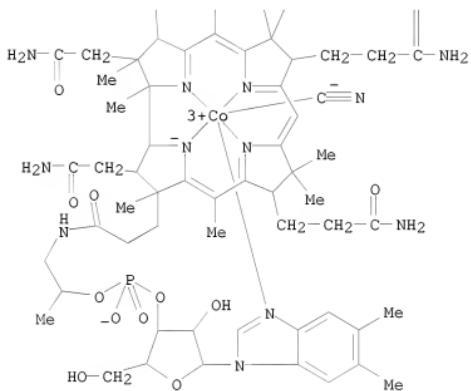


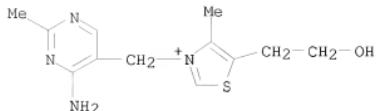
CM 3

Absolute stereochemistry.



CM 4



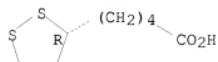


● Cl⁻

L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Arginine, (3R)-1,2-dithiolane-3-pentanoate (9CI)
 MF C8 H14 O2 S2 . x C6 H14 N4 O2

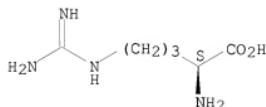
CM 1

Absolute stereochemistry. Rotation (+).



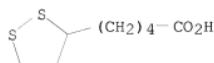
CM 2

Absolute stereochemistry.



L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Adenosine, 5'--[[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-,
 1,3-propanedisulfonate (1:1) (salt), mixt. with 1,2-dithiolane-3-pentanoic
 acid (9CI)
 MF C15 H23 N6 O5 S . C8 H14 O2 S2 . C3 H7 O6 S2
 CI MXS

CM 1



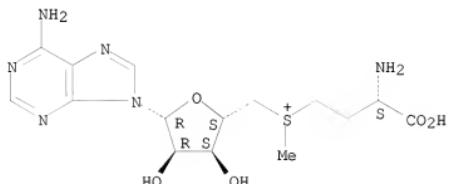
CM 2

CM 3

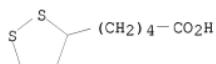


CM 4

Absolute stereochemistry.



L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,2-Dithiolane-3-pentanoic acid, magnesium salt (2:1)
MF C8 H14 O2 S2 . 1/2 Mg
CI COM

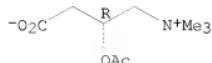


● 1/2 Mg

L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1-Propanaminium, 2-(acetyloxy)-3-carboxy-N,N,N-trimethyl-, inner salt,
(2R)-, mixt. with (3R)-1,2-dithiolane-3-pentanoic acid
MF C9 H17 N O4 . C8 H14 O2 S2
CI MXS

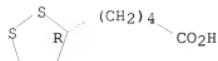
CM 1

Absolute stereochemistry.



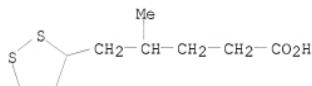
CM 2

Absolute stereochemistry. Rotation (+).

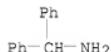


L3 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,2-Dithiolane-3-valeric acid, γ -methyl-, compd. with
1,1-diphenylmethyldiamine (7CI)
MF C13 H13 N . C9 H16 O2 S2

CM 1



CM 2



ALL ANSWERS HAVE BEEN SCANNED

=> logogoff hold
0 LOGOGOFF
39 HOLD
L4 0 LOGOGOFF HOLD
(LOGOGOFF (W) HOLD)

=> logoff hold
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 25.43 25.85

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 15:00:25 ON 18 JUN 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * * Welcome to STN International * * * * * * * * * * *

NEWS 1 JAN 02 Web Page for STN Seminar Schedule - N. America
NEWS 2 JAN 02 STN pricing information for 2008 now available
NEWS 3 JAN 16 CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 4 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 5 JAN 28 MARPAT searching enhanced
NEWS 6 JAN 28 USGENE now provides USPTO sequence data within 3 days of publication
NEWS 7 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 8 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements
NEWS 9 FEB 08 STN Express, Version 8.3, now available
NEWS 10 FEB 20 PCI now available as a replacement to DPCI
NEWS 11 FEB 25 IFIREF reloaded with enhancements
NEWS 12 FEB 25 IMSPRODUCT reloaded with enhancements
NEWS 13 FEB 29 WPINDEX/WPIIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS 14 MAR 31 IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS 15 MAR 31 CAS REGISTRY enhanced with additional experimental spectra
NEWS 16 MAR 31 CA/CAPlus and CASREACT patent number format for U.S. applications updated
NEWS 17 MAR 31 LPCI now available as a replacement to LDPCI
NEWS 18 MAR 31 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 19 APR 04 STN AnaVist, Version 1, to be discontinued
NEWS 20 APR 15 WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS 21 APR 28 EMBASE Controlled Term thesaurus enhanced
NEWS 22 APR 28 IMSRESEARCH reloaded with enhancements
NEWS 23 MAY 30 INFAPAMDB now available on STN for patent family searching
NEWS 24 MAY 30 DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS 25 JUN 06 EPFULL enhanced with 260,000 English abstracts
NEWS 26 JUN 06 KOREPAT updated with 41,000 documents
NEWS 27 JUN 13 USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 05:26:27 ON 19 JUN 2008

```
=> file reg  
COST IN U.S. DOLLARS  
SINCE FILE ENTRY TOTAL  
FULL ESTIMATED COST 0.21 SESSION 0.21
```

FILE 'REGISTRY' ENTERED AT 05:26:41 ON 19 JUN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 18 JUN 2008 HIGHEST RN 1029146-45-9
DICTIONARY FILE UPDATES: 18 JUN 2008 HIGHEST RN 1029146-45-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

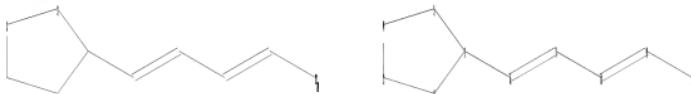
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

```
=>  
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary  
files\10025947\10025947 thioctic diene.str
```



```
chain nodes :  
6 7 8 9 10  
ring nodes :  
1 2 3 4 5  
chain bonds :  
1-6 6-7 7-8 8-9 9-10  
ring bonds :  
1-2 1-5 2-3 3-4 4-5  
exact/norm bonds :  
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exact bonds :  
1-6 6-7 7-8 8-9 9-10
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Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
10:CLASS
```

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

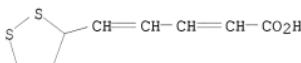
=> search l1 exact full
FULL SEARCH INITIATED 05:27:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L2 2 SEA EXA FUL L1

=> d scan 1-2
'1-2' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

L2 2 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2,4-Pentadienoic acid, 5-(1,2-dithiolan-3-yl)-
MF C8 H10 O2 S2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

| | |
|--------|---|
| REG | - RN |
| SAM | - Index Name, MF, and structure - no RN |
| FIDE | - All substance data, except sequence data |
| IDE | - FIDE, but only 50 names |
| SQIDE | - IDE, plus sequence data |
| SQIDE3 | - Same as SQIDE, but 3-letter amino acid codes are used |
| SQD | - Protein sequence data, includes RN |
| SQD3 | - Same as SQD, but 3-letter amino acid codes are used |
| SQN | - Protein sequence name information, includes RN |
| CALC | - Table of calculated properties |

EPROP -- Table of experimental properties
PROP -- EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

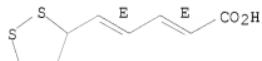
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 2 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2,4-Pentadienoic acid, 5-(1,2-dithiolan-3-yl)-, (E,E)- (9CI)
MF C8 H10 O2 S2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE
ENTRY
60.77
TOTAL
SESSION
60.98

FILE 'CAPLUS' ENTERED AT 05:27:57 ON 19 JUN 2008
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE LAST UPDATED: 18 Jun 2008 (20080618/ED)

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They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> l2
L3 1 L2
=> d l3 ti fbib abs

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
TI 1,2-Dithiol-3-ylpropenoic acid and -pentadienoic acid derivatives
AN 1987:176369 CAPLUS
DN 106:176369
OREF 106:28629a,28632a
TI 1,2-Dithiol-3-ylpropenoic acid and -pentadienoic acid derivatives
IN Yamamoto, Itaru; Matsubara, Akira; Yamashita, Hiroyuki; Mizuno, Osamu;
Sakaguchi, Mitsuhiro; Kumakura, Mikio
PA Mitsui Toatsu Chemicals, Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 17 pp.

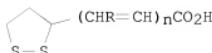
CODEN: JKXXAF

DT Patent
LA Japanese

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|-------------|------|----------|-----------------|----------|
| PI | JP 62022779 | A | 19870130 | JP 1985-161158 | 19850723 |
| | JP 05072389 | B | 19931012 | JP 1985-161158 | 19850723 |

GI



I

AB The title compds. (I; n = 1, 2; R = H, Me) and physiol. acceptable salts, useful as immunomodulators, are prepared Reaction of 4-formyl-2,2-dimethyl-1,3-dithiane with Ph3P:CHCO₂Et in benzene followed by saponification and oxidation

with H₂O₂ in MeOH in the presence of Na₂WO₄ gave (E)-3-(2,2-dimethyl-1-oxo-1,3-dithian-4-yl)acrylic acid whose ring contraction in dioxane containing 6N H₂SO₄ at 95° gave 76% (E)-I (n = 1, R = H). I in vitro were more effective as immunostimulants than lipoic acid in BALB/C mouse spleen cells stimulated by a T cell mitogen, concanavalin A.

| | | | |
|--|------------------|---------------|--|
| => file reg | | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION | |
| FULL ESTIMATED COST | 5.31 | 66.29 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION | |
| CA SUBSCRIBER PRICE | -0.80 | -0.80 | |

FILE 'REGISTRY' ENTERED AT 05:30:43 ON 19 JUN 2008
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STRUCTURE FILE UPDATES: 18 JUN 2008 HIGHEST RN 1029146-45-9
DICTIONARY FILE UPDATES: 18 JUN 2008 HIGHEST RN 1029146-45-9

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10025947\10025947 thictic alkene 1.str



chain nodes :
6 7 8 9 10
ring nodes :
1 2 3 4 5
chain bonds :
1-6 6-7 7-8 8-9 9-10

ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
1-6 6-7 7-8 8-9 9-10

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

L4 STRUCTURE UPLOADED

=> d 14
L4 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.

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FULL SEARCH INITIATED 05:31:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L5 0 SEA EXA FUL L4

=>
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary
files\10025947\10025947 2nd thietic alkene.str



chain nodes :
6 7 8 9 10
ring nodes :
1 2 3 4 5
chain bonds :
1-6 6-7 7-8 8-9 9-10
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :

1-6 6-7 7-8 8-9 9-10

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

L6 STRUCTURE UPLOADED

=> d 16
L6 HAS NO ANSWERS
L6 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 16 exact full
FULL SEARCH INITIATED 05:32:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L7 0 SEA EXA FUL L6

=> logoff hold
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
CA SUBSCRIBER PRICE ENTRY SESSION
0.00 -0.80

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 05:33:07 ON 19 JUN 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPSTA1623PAZ

PASSWORD:
* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 05:35:44 ON 19 JUN 2008
FILE 'REGISTRY' ENTERED AT 05:35:44 ON 19 JUN 2008
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| | | |
|--|------------------|----------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL |
| FULL ESTIMATED COST | 121.54 | SESSION 187.83 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL |
| CA SUBSCRIBER PRICE | 0.00 | SESSION -0.80 |

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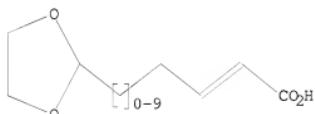


chain nodes :
6 7 8 9 10
ring nodes :
1 2 3 4 5
chain bonds :
1-6 6-7 7-8 8-9 9-10
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
1-6 6-7 7-8 8-9 9-10

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

L8 STRUCTURE UPLOADED

=> d 18
L8 HAS NO ANSWERS
L8 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 18 sss sam
SAMPLE SEARCH INITIATED 05:36:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED
SEARCH TIME: 00.00.01

8 ITERATIONS

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8 TO 329
PROJECTED ANSWERS: 0 TO 0

L9 0 SEA SSS SAM L8

=> search 18 sss full
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FULL SCREEN SEARCH COMPLETED - 180 TO ITERATE

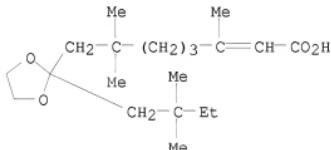
100.0% PROCESSED
SEARCH TIME: 00.00.01

180 ITERATIONS
12 ANSWERS

L10 12 SEA SSS FUL L8

=> d scan

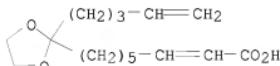
L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Octenoic acid, 8-[2-(2,2-dimethylbutyl)-1,3-dioxolan-2-yl]-3,7,7-
trimethyl-
MF C20 H36 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

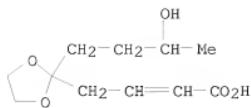
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):12

L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Octenoic acid, 8-[2-(4-pentenyl)-1,3-dioxolan-2-yl]- (9CI)
MF C16 H26 O4



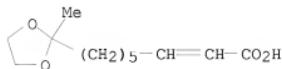
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[2-(3-hydroxybutyl)-1,3-dioxolan-2-yl]-
MF C11 H18 O5



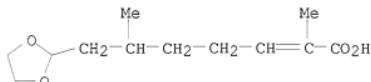
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Octenoic acid, 8-(2-methyl-1,3-dioxolan-2-yl)-
MF C12 H20 O4



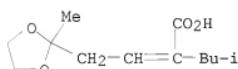
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Heptenoic acid, 7-(1,3-dioxolan-2-yl)-2,6-dimethyl-
MF C12 H20 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

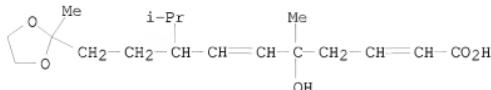
L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Pentanoic acid, 4-methyl-2-[2-(2-methyl-1,3-dioxolan-2-yl)ethylidene]-
IN C12 H20 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2,6-Decadienoic acid, 5-hydroxy-5,9-dimethyl-8-[2-(2-methyl-1,3-dioxolan-2-

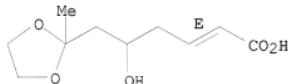
yl)ethyl-
MF C18 H30 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Hexenoic acid, 5-hydroxy-6-(2-methyl-1,3-dioxolan-2-yl)-, (E)- (9CI)
MF C10 H16 O5

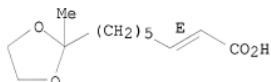
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Octenoic acid, 8-(2-methyl-1,3-dioxolan-2-yl)-, (E)- (9CI)
MF C12 H20 O4

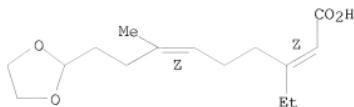
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2,6-Nonadienoic acid, 9-(1,3-dioxolan-2-yl)-3-ethyl-7-methyl-, (Z,Z)- (9CI)
MF C15 H24 O4

Double bond geometry as shown.

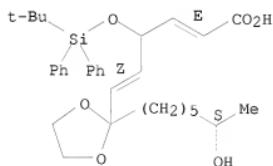


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2,5-Hexadienoic acid, 4-[(1,1-dimethylethyl)diphenylsilyloxy]-6-[2-[(6S)-6-hydroxyheptyl]-1,3-dioxolan-2-yl]-, (2E,5Z)-
 MF C32 H44 O6 Si

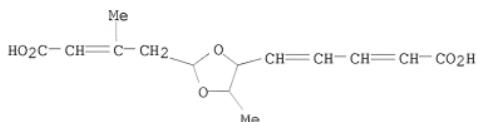
Absolute stereochemistry.

Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2,4-Pentadienoic acid, 5-[2-(3-carboxy-2-methyl-2-propenyl)-5-methyl-1,3-dioxolan-4-yl]- (9CI)
 MF C14 H18 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> e 2-Octenoic acid, 8-(2-methyl-1,3-dioxolan-2-yl)-/cn
 E1 1 2-OCTENOIC ACID, 8-(2-FORMYLPHENYL)-2-METHYL-, ETHYL ESTER/C

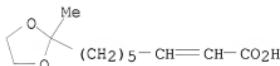
E2 1 2-OCTENOIC ACID, 8-(2-FORMYLPHENYL)-2-METHYL-, ETHYL ESTER,
 (E)-/CN
 E3 1 --> 2-OCTENOIC ACID, 8-(2-METHYL-1,3-DIOXOLAN-2-YL)-/CN
 E4 1 2-OCTENOIC ACID, 8-(2-METHYL-1,3-DIOXOLAN-2-YL)-, (E)-/CN
 E5 1 2-OCTENOIC ACID, 8-(2-METHYL-1,3-DIOXOLAN-2-YL)-, ETHYL ESTER,
 (E)-/CN
 E6 1 2-OCTENOIC ACID, 8-(2-METHYL-1,3-DIOXOLAN-2-YL)-, METHYL ESTER/CN
 E7 1 2-OCTENOIC ACID, 8-(2-METHYL-1,3-DIOXOLAN-2-YL)-, METHYL ESTER,
 (E)-/CN
 E8 1 2-OCTENOIC ACID, 8-(2-OXO-1(2H)-PYRIDINYL)-, ETHYL ESTER, (E)
)-/CN
 E9 1 2-OCTENOIC ACID, 8-(2-PYRIDYL)-/CN
 E10 1 2-OCTENOIC ACID, 8-(2H-BENZOTRIAZOL-2-YL)-8-(4-MORPHOLINYLYL)-
 , ETHYL ESTER, (E)-/CN
 E11 1 2-OCTENOIC ACID, 8-(2H-BENZOTRIAZOL-2-YL)-8-(BIS(PHENYLMETHYL)AMINO)-,
 ETHYL ESTER, (E)-/CN
 E12 1 2-OCTENOIC ACID, 8-(3,3-DIMETHYLOXIRANYL)-3,6-DIMETHYL-, ETHYL ESTER/CN

=> e3

L11 1 "2-OCTENOIC ACID, 8-(2-METHYL-1,3-DIOXOLAN-2-YL)-"/CN

=> d 111

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
 RN 96181-65-6 REGISTRY
 ED Entered STN: 04 May 1985
 CN 2-Octenoic acid, 8-(2-methyl-1,3-dioxolan-2-yl)- (CA INDEX
 NAME)
 MF C12 H20 O4
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

| | | | |
|--|------------|---------|--|
| => file caplus | | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL | |
| | ENTRY | SESSION | |
| FULL ESTIMATED COST | 308.89 | 375.18 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL | |
| | ENTRY | SESSION | |
| CA SUBSCRIBER PRICE | 0.00 | -0.80 | |

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FILE LAST UPDATED: 18 Jun 2008 (20080618/ED)

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```
=> l11
L12      1 L11

=> d l12 ti fbib abs

L12 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
TI New syntheses of queen substance and trans-9-hydroxy-2-decenoic acid
AN 1963:46309 CAPLUS
DN 58:46309
OREF 58:7821e-h,7822a-g
TI New syntheses of queen substance and trans-9-hydroxy-2-decenoic acid
AU Eiter, Karl
CS Farbenfabriken Bayer A.-G., Leverkusen, Germany
SO Justus Liebigs Annalen der Chemie (1962), 658, 91-9
CODEN: JLACBF; ISSN: 0075-4617
DT Journal
LA Unavailable
OS CASREACT 58:46309
AB cf. CA 57, 9658c. The queen bee secretion, trans-9-oxo-2-decenoic acid
(I) was synthesized from OHC(CH2)3CHO (II). Freshly distilled II (1.39 mole)
stirred (N atmospheric) with portionwise addition of dry powdered Ph3P:CHCO2Me
(0.69
mole) with rising temperature to 80°, and the mixture kept 1.5 hrs. at
80-90°, the cooled mixture diluted with 130 ml. Et2O and cooled to
-20°, filtered from residual Ph3P, and the filtrate and petr.
ether washings evaporated, the residual oil fractionally distilled to give II,
b0.08 65°, and 90 g. product, b0.08 65-122°, and the product
rectified gave 7.56 g. material, b0.12 54-60°, n20D 1.4400; 56.5 g.
cis,trans-OHC(CH2)3CH:CHCO2Me (III), b0.09 60-75°, n20D 1.4590, v
2945, 2730, 1736, 1663, 987, 854, 826 cm.-1, [2,4-dinitrophenylhydrazone
m. 85° (alc.)] and 25.94 g. III, b0.08 75-100°, n20D
1.4664. Al flakes (13.2 g., activated with HgCl2 and trace of iodine)
stirred (H2O-free N atmospheric) in 90 ml. absolute tetrahydrofuran at 60°
with careful dropwise addition of 85.2 g. HC.tplbond.CCH2Br in 84 ml. absolute
tetrahydrofuran, vigorously stirred at -50° with dropwise addition of
114 g. III in 120 ml. tetrahydrofuran, and the mixture stirred 1 hr. at
0°, decomposed with saturated aqueous NH4Cl, and extracted with Et2O, the
neutral
NaCl-washed and dried extract evaporated, and the oil (136.0 g.) distilled
yielded
95% HC.tplbond.CCH2CH(OH)(CH2)3CH:CHCO2Me (IV), b0.001, 105-8°,
```

n_{20D} 1.4860, ν 3510, 3290, 2120, 1730, 1666, 986, 853 cm.⁻¹ Zn dust (9.2 g., activated with iodine) stirred (N atmospheric) in 14 ml. 1:6 tetrahydrofuran-Et₂O with addition of 14.4 g. HC.tpbond.CCH₂Br and 15.8 g. III in 30 ml. 1:2 tetrahydrofuran-absolute Et₂O, the mixture stirred 15 min. with gentle heating, and the cooled mixture decomposed with saturated aqueous NaCl and extracted with Et₂O gave 18.9 g. material, distilled in a high vacuum to yield 58% IV, n_{20D} 1.4862, ν 3510, 3280, 2115, 1950, 1729, 1663, 984, 852 cm.⁻¹, containing a small amount of allene compound IV (81.3 g.) in 500 ml. dioxane stirred (N atmospheric) under reflux with 1.5 g. basic HgSO₄ and boiled 10 min. with dropwise addition of 100 ml. 20% H₂SO₄, the cooled mixture saturated with NaCl and extracted with Et₂O, the extract shaken with saturated aqueous NaCl and the dried filtered extract evaporated, the residue (90.2 g.) chromatographed from 1:1 petr. ether-C₆H₆ on Al₂O₃ (activity II), and fractions 1-3 combined gave 67% AcCH:CH(CH₂)₃CH:CHCO₂Me (V), b_{0.19} 110-12°, n_{20D} 1.4857, ν 1728, 1680, 1636, 1440, 980 cm.⁻¹ III (50 g.) in 100 ml. pure Me₂CO treated with 10 g. piperidine and 8 g. AcOH and the mixture refluxed (N atmospheric) 1 hr., excess Me₂CO evaporated in vacuo, and the residue extracted with Et₂O, the product (40 g.) chromatographed from 1:1 petr. ether-C₆H₆ on Al₂O₃, and the substance (31 g., b_{0.001} 80-130°) fractionated gave 1.4 g. fraction, b_{0.001} 111-15°, n_{20D} 1.4818; 4.1 g. fraction, b_{0.001} 115-19°, n_{20D} 1.4866; 3.4 g. fraction, b_{0.001} 119-30°, n_{20D} 1.4908; and 1.1 g. fraction, b_{0.001} 130-7°, n_{20D} 1.4992. The 1st 3 fractions had bands at ν 1720, 1678, 1629, 1430, and 980 cm.⁻¹, practically identical with those of V. V (37.7 g., obtained by ketonization) in 130 ml. MeOH hydrogenated 10 hrs. with 0.8 g. 5% Pd-CaCO₃ (poisoned with 1.6 mg. Pb(OAc)₄ and prerduced in 30 ml. MeOH) and the product distilled yielded 80% Ac(CH₂)₅CH:CHCO₂Me (VI), n_{20D} 1.425, ν 1720, 1708, 1658, 980 cm.⁻¹ V (10.55 g., prepared by Knoevenagel condensation) in 30 ml. MeOH added to 0.3 g. prerduced Lindlar catalyst in 20 ml. MeOH and the mixture hydrogenated 7.33 hrs., filtered, and the residue on evaporation distilled in a bulb tube gave 10.5 g. VI, b_{0.001} 80-100°, n_{20D} 1.4590. I (500 mg.) in 10 ml. absolute Et₂O at 0° treated with titrated CH₂N₂ in Et₂O, the mixture kept 30 min. before shaking with aqueous Na₂CO₃ and H₂O, drying, and evaporating, and the oily residue distilled gave VI, b_{0.001} 75-90°, n_{20D} 1.4495. VI (30.4 g.) in 120 ml. dioxane autoclaved 1 hr. at 150° with 210 ml. 2N Na₂CO₃ and the mixture freed from dioxane in vacuo, diluted with H₂O, and freed from 0.3 g. VI by extraction with Et₂O, the aqueous phase saturated with NaCl and extracted with Et₂O, the oily product (24.5 g.) distilled at 115-55°/ 0.001 mm. and the crystalline product (10.5 g.) recrystd. at 0° from Et₂O-petr. ether gave I, Ac(CH₂)₅CH:CHCO₂H, m. 51-3°, λ 214 $\mu\mu$ (e 11,700). The mother liquor gave an oily acid, n_{20D} 1.4675, which, chromatographed on silica gel and eluted with 4:1 C₆H₆-Et₂O, gave cis-9-oxo-2-decenoic acid (cis-VII), b_{0.001} 120-30°, n_{20D} 1.4685, ν 3030, 2930, 2848, 2675, 1710, 1652, 1461, 1424, 1363, 1287, 1223, 1174, 1093, 1031, 994, 830, 721 cm.⁻¹, together with 1, n_{20D} 1.4700. VII (15.5 g.) in 200 ml. C₆H₆ refluxed 8 hrs. with 30 g. HOCH₂CH₂OH and 300 mg. p-MeC₆H₄SO₃H under a Dean-Stark head and the product extracted with Et₂O gave 18.3 g. VII ethylene ketal, b_{0.001} 100-20°, n_{20D} 1.4650, ν 1720, 1652, 1437, 1063, 1040, 980, 946, 719 cm.⁻¹ VII (5g.) refluxed 1 hr. in 25 ml. 25% NaOH, the cooled mixture washed with Et₂O, and the aqueous phase acidified at 0° with HCl to pH 3 and extracted with Et₂O gave 4 g. oily ethylene ketal (VIII) of VII, b_{0.001} 115-35°, n_{20D} 1.4748, ν 3100, 1705, 1652, 1420, 1063, 1043, 981, 946, 720 cm.⁻¹ VIII (11.9 g.) in

150 ml. purest dioxane refluxed 30 min. with 12 ml. 2N HCl and the mixture freed from solvent, the residue taken up in Et2O, and the residue on evaporation distilled at 120-40°/0.001 ml. gave a colorless viscous oil, crystallized from Et2O-petr. ether to give 4.2 g. VII. I (4 g., m. 52-3°) treated at 0° in 60 ml. absolute C6H6 (atmospheric) with 8 ml. SOC12 in 32 ml. petr. ether, the mixture heated gradually to room temperature

and

finally to boiling, treated dropwise with 1.6 ml. SOC12 in 12 ml. petr. ether, and the mixture refluxed 1 hr., the cooled mixture freed carefully from solvent in vacuo, and the residue distd; gave 2.9 g. yellow-green oily trans-MeCO(CH2)5CH:CHCOCl (IX), b0.001 110-40°, n20D 1.4775, v 2925, 2840, 1790, 1760, 1709, 1622, 1462, 1415, 1358, 1296, 1279, 1160, 1118, 1097, 1052, 971, 917, 767, 748, 721, 679 cm.-1 Oily I (14.8 g., from queen substance mother liquors) in 220 ml. absolute C6H6 at 0° treated with 30 ml. SOC12 in 120 ml. petr. ether, the mixture kept 1 hr. at 50°, the solvent evaporated in vacuo, and the acid chloride (b0.001 110-25°, n20D 1.4779) stirred in 30 ml. dioxane with dropwise addition of 150 ml. 2N Na2CO3, the mixture stirred 6 hrs. at 20° and kept 16 hrs., the alkaline aqueous phase washed with Et2O and acidified with 2N HCl, saturated with NaCl, and extracted with Et2O gave 12.6 g. acid, b0.001 110-40°, crystallized from Et2O-petr. ether at 0° to give 3.8 g. crystals, m. 39.5-41.5°, recrystd. 3 times to give a little I, m. 51-4°.

A noteworthy isomerization of cis- to trans-I was not established. 1 (11.04 g., m. 51°) in 80 ml. MeOH stirred at 20° with portionwise addition of 3.6 g. KBH4 and the mixture heated 30 min. on a steam bath, the residue on evaporation taken up in H2O and adjusted at 0° (ice bath) to pH 3 with 2N H2SO4, saturated with NaCl, and repeatedly extracted with Et2O gave 11.8 g. acid, n20D 1.4737, distilled at 120-40°/0.001 ml. and the colorless oil, n20D 1.4761, crystallized at 0° from Et2O-petr. ether gave waxy trans-9-hydroxy-2-decenic acid, m. 43-5°, v 3080, 2945, 2680, 1715, 1655, 1465, 1423, 1365, 1315, 1295, 1220, 1175, 1110, 981, 938, 812, 723 cm.-1, identical with the royal jelly of Brown and Felauer (CA 55, 17916b).

=> logoff hold
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| | SINCE FILE | TOTAL |
|--|------------|---------|
| | ENTRY | SESSION |

| | |
|-------|--------|
| 10.59 | 385.77 |
|-------|--------|

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| | SINCE FILE | TOTAL |
|--|------------|---------|
| | ENTRY | SESSION |

CA SUBSCRIBER PRICE

| | |
|-------|-------|
| -0.80 | -1.60 |
|-------|-------|

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 05:48:15 ON 19 JUN 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPATA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 05:56:34 ON 19 JUN 2008
FILE 'CAPLUS' ENTERED AT 05:56:34 ON 19 JUN 2008
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

| | | |
|--|------------------|---------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 10.59 | 385.77 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -0.80 | -1.60 |
| => file reg | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 10.59 | 385.77 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -0.80 | -1.60 |

FILE 'REGISTRY' ENTERED AT 05:56:47 ON 19 JUN 2008
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
 provided by InfoChem.

STRUCTURE FILE UPDATES: 18 JUN 2008 HIGHEST RN 1029146-45-9
 DICTIONARY FILE UPDATES: 18 JUN 2008 HIGHEST RN 1029146-45-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

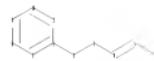
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
 Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary
 files\10025947\10025947 pneyl substituted enoic acid.str



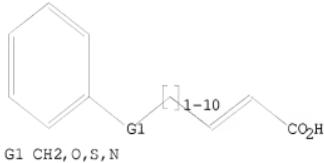
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2 3 4 5 6
ring nodes :
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chain bonds :
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exact/norm bonds :
1-2 2-3
exact bonds :
3-4 4-5 5-6
normalized bonds :
1-7 1-11 7-8 8-9 9-10 10-11
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G1:CH2,O,S,N

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS

L13 STRUCTURE UPLOADED

=> d 113
L13 HAS NO ANSWERS
L13 STR



G1 CH₂, O, S, N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 7483 TO ITERATE

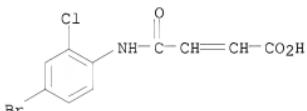
26.7% PROCESSED 2000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 144474 TO 154846
PROJECTED ANSWERS: 5153 TO 7267

L14 50 SEA SSS SAM L13

=> d scan

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(4-bromo-2-chlorophenyl)amino]-4-oxo-
MF C10 H7 Br Cl N O3

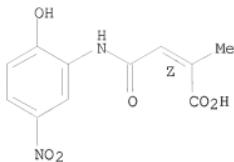


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

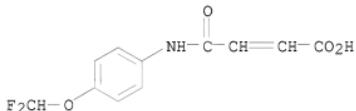
L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(2-hydroxy-5-nitrophenyl)amino]-2-methyl-4-oxo-, (2Z)-
MF C11 H10 N2 O6

Double bond geometry as shown.



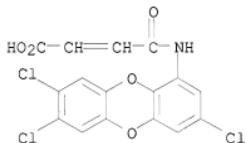
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(4-(difluoromethoxy)phenyl)amino]-4-oxo-
 MF C11 H9 F2 N O4



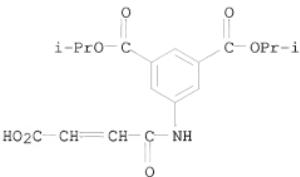
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-oxo-4-[(3,7,8-trichlorodibenzo[b,e][1,4]dioxin-1-yl)amino]-
 MF C16 H8 Cl13 N O5



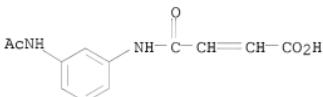
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 1,3-Benzenedicarboxylic acid, 5-[(3-carboxy-1-oxo-2-propen-1-yl)amino]-,
 1,3-bis(1-methylethyl) ester
 MF C18 H21 N O7



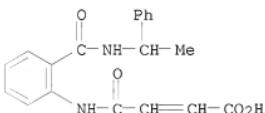
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(3-(acetylamino)phenyl)amino]-4-oxo-
 MF C12 H12 N2 O4



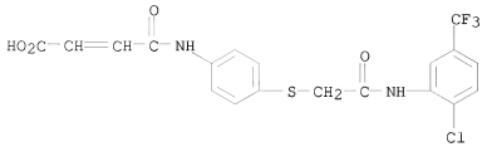
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-oxo-4-[(2-[(1-phenylethyl)amino]carbonyl)phenyl]amino-
 MF C19 H18 N2 O4



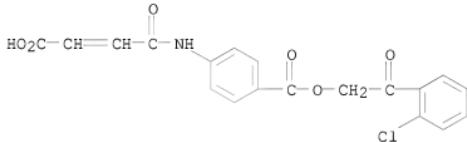
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(4-[(2-chloro-5-(trifluoromethyl)phenyl)amino]-2-
 oxoethyl)thio]phenylamino-4-oxo-
 MF C19 H14 Cl F3 N2 O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

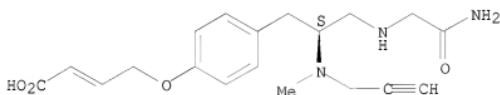
L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Benzoic acid, 4-[(3-carboxy-1-oxo-2-propen-1-yl)amino]-,
 1-[2-(2-chlorophenyl)-2-oxoethyl] ester
 MF C19 H14 Cl N O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

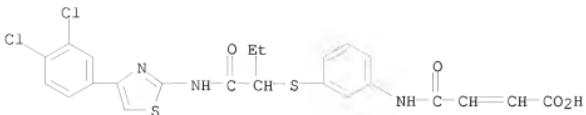
L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(2S)-3-[(2-amino-2-oxoethyl)amino]-2-(methyl-2-
 propyn-1-ylamino)propyl]phenoxy]-
 MF C19 H25 N3 O4

Absolute stereochemistry.
 Double bond geometry unknown.



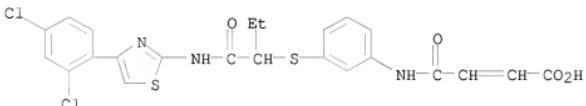
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN INDEX NAME NOT YET ASSIGNED
 MF C23 H19 C12 N3 O4 S2



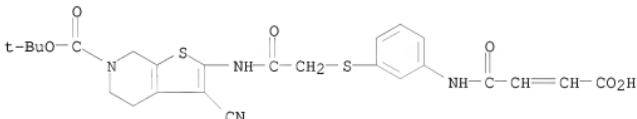
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN INDEX NAME NOT YET ASSIGNED
 MF C23 H19 C12 N3 O4 S2



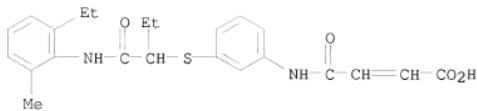
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Thieno[2,3-c]pyridine-6(5H)-carboxylic acid, 2-[(2-[(3-[(3-carboxy-1-oxo-2-propen-1-yl)amino]phenyl)thio]acetyl)amino]-3-cyano-4,7-dihydro-,
 6-(1,1-dimethylethyl) ester
 MF C25 H26 N4 O6 S2



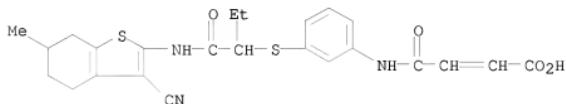
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN INDEX NAME NOT YET ASSIGNED
 MF C23 H26 N2 O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

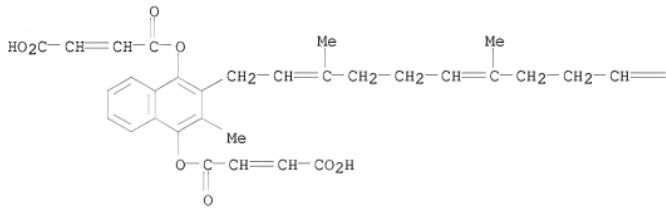
L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C24 H25 N3 Q4 S2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenedioic acid (2E)-, 2-methyl-3-[(2E,6E,10E)-3,7,11,15-tetramethyl-
2,6,10,14-hexadecatetraenyl]-1,4-naphthalenediyl ester (9CI)
MF C39 H46 O8
CI COM

PAGE 1-A



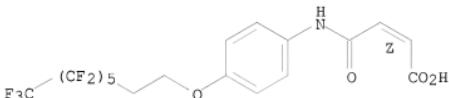
PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-oxo-4-[4-[(3,3,4,4,5,5,6,6,7,7,8,8,8-
tridecafluoroctyl)oxyl]phenyl]amino]-, (Z)- (9CI)
MF C18 H12 F13 N O4

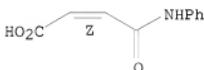
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-oxo-4-(phenylamino)-, antimony(3+) salt (3:1), (Z)-
(9CI)
MF C10 H9 N O3 . 1/3 Sb

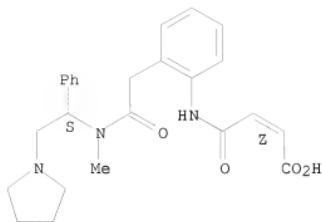
Double bond geometry as shown.



●1/3 Sb(III)

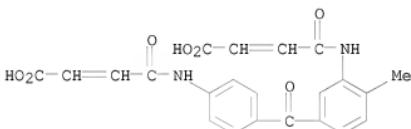
L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[[2-[2-[methyl[(1S)-1-phenyl-2-(1-
pyrrolidinyl)ethyl]amino]-2-oxoethyl]phenyl]amino]-4-oxo-, (2Z)-
MF C25 H29 N3 O4
CI COM

Absolute stereochemistry.
Double bond geometry as shown.



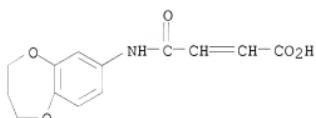
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(5-[(4-[(3-carboxy-1-oxo-2-propen-1-yl)amino]benzoyl]-2-methylphenyl)amino]-4-oxo-
 MF C22 H18 N2 O7



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

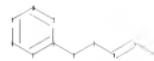
L14 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(3,4-dihydro-2H-1,5-benzodioxepin-7-yl)amino]-4-oxo-
 MF C13 H13 N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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 Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10025947\10025947 phenyl substituted enoic.acid.str



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2 3 4 5 6
ring nodes :
1 7 8 9 10 11
chain bonds :
1-2 2-3 3-4 4-5 5-6
ring bonds :
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exact/norm bonds :
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1-7 1-11 7-8 8-9 9-10 10-11

G1:CH2,O,S,N

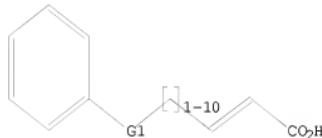
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3:>= minimum 2
Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS

L15 STRUCTURE UPLOADED

=> d 115

L15 HAS NO ANSWERS

L15 STR



G1 CH₂,O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> search 115 sss sam

SAMPLE SEARCH INITIATED 06:00:58 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 7483 TO ITERATE

26.7% PROCESSED 2000 ITERATIONS

4 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 144474 TO 154846

PROJECTED ANSWERS: 67 TO 531

L16 4 SEA SSS SAM L15

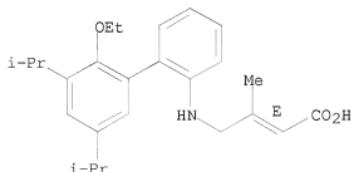
=> d scan

L16 4 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2-Butenoic acid, 4-[(2'-ethoxy-3',5'-bis(1-methylethyl)[1,1'-biphenyl]-2-yl)amino]-3-methyl-, (2E)-

MF C₂₅ H₃₃ N O₃

Double bond geometry as shown.

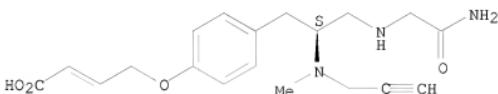


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

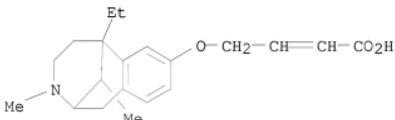
L16 4 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[4-[(2S)-3-[(2-amino-2-oxoethyl)amino]-2-(methyl-2-propyn-1-ylamino)propyl]phenoxy]-
MF C19 H25 N3 O4

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

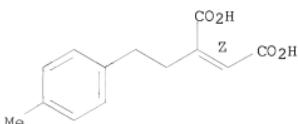
L16 4 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(6-ethyl-1,2,3,4,5,6-hexahydro-3,11-dimethyl-2,6-methano-3-benzazocin-8-yl)oxy]-
MF C20 H27 N O3
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 4 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Maleic acid, (p-methylphenethyl)- (6CI)
MF C13 H14 O4

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

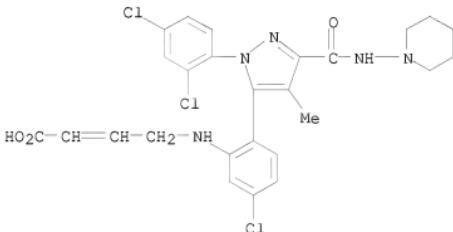
=> search l15 sss full
FULL SEARCH INITIATED 06:02:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 149714 TO ITERATE

100.0% PROCESSED 149714 ITERATIONS 404 ANSWERS
SEARCH TIME: 00.00.01

L17 404 SEA SSS FUL L15

=> d scan

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[[5-chloro-2-[1-(2,4-dichlorophenyl)-4-methyl-3-[(1-piperidinylamino)carbonyl]-1H-pyrazol-5-yl]phenyl]amino]-
MF C26 H26 C13 N5 O3

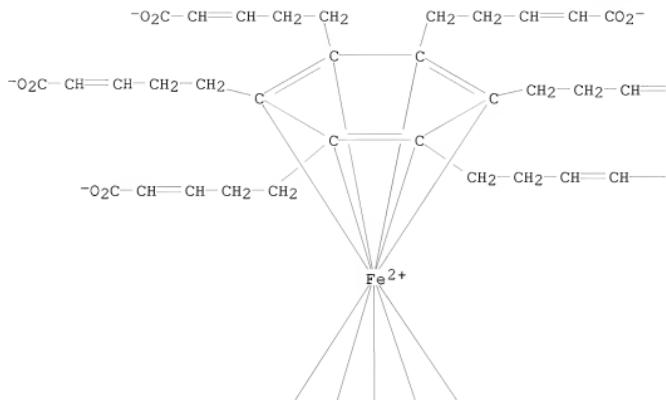


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Ferrate(5-), [(2E,2'E,2''E,2'''E,2''''E)-5,5',5'',5'',5''',5''''-(n6-1,2,3,4,5,6-benzenehexayl)hexakis[2-pentenoato]l(6-)](n5-2,4-cyclopentadien-1-yl)- (9CI)
MF C41 H41 Fe O12
CI CCS, COM

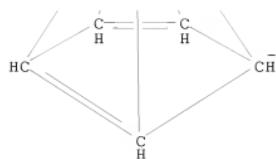
PAGE 1-A



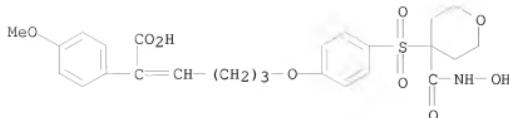
PAGE 1-B



PAGE 2-A



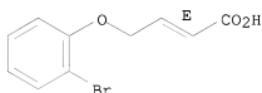
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Benzeneacetic acid, 4-methoxy- α -[4-[4-[[tetrahydro-4-
[(hydroxyamino)carbonyl]-2H-pyran-4-yl]sulfonyl]phenoxy]butylidene]-
MF C25 H29 N O9 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

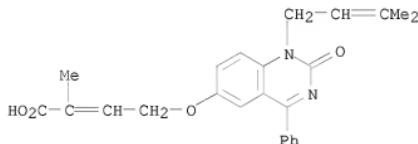
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-(2-bromophenoxy)-, (E)- (9CI)
 MF C10 H9 Br O3

Double bond geometry as shown.



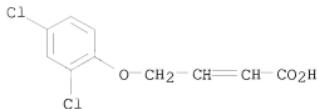
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[1,2-dihydro-1-(3-methyl-2-butenoil)-2-oxo-4-phenyl-6-quinazolinyl]oxy]-2-methyl- (9CI)
 MF C24 H24 N2 O4



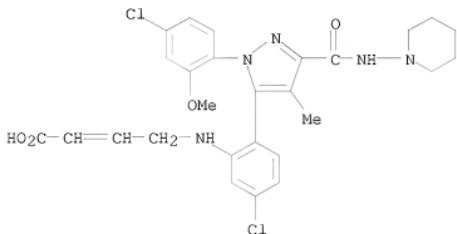
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-(2,4-dichlorophenoxy)-
 MF C10 H8 Cl2 O3
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

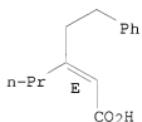
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(5-chloro-2-methoxyphenyl)-4-methyl-3-[(1-piperidinylamino)carbonyl]-1H-pyrazol-5-yl]phenyl]amino-
 MF C27 H29 Cl2 N5 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

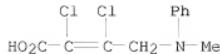
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Hexenoic acid, 3-(2-phenylethyl)-, (2E)-
 MF C14 H18 O2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

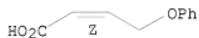
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 2,3-dichloro-4-(methylphenylamino)-
 MF C11 H11 Cl2 N O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-phenoxy-, (Z)- (9CI)
MF C10 H10 O3

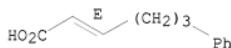
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

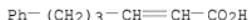
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Hexenoic acid, 6-phenyl-, (2E)-
MF C12 H14 O2

Double bond geometry as shown.



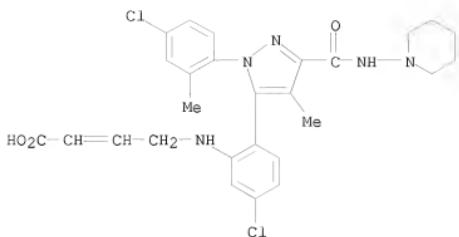
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Hexenoic acid, 6-phenyl-
MF C12 H14 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

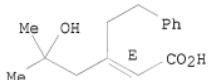
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(5-chloro-2-[1-(4-chloro-2-methylphenyl)-4-methyl-3-[(1-piperidinylamino)carbonyl]-1H-pyrazol-5-yl]phenyl]amino]-
MF C27 H29 Cl2 N5 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Hexenoic acid, 5-hydroxy-5-methyl-3-(2-phenylethyl)-, (2E)-
 MF C15 H20 O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

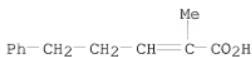
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Hexenoic acid, 6-phenyl-, (2Z)-
 MF C12 H14 O2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

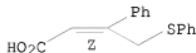
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Pentenoic acid, 2-methyl-5-phenyl-, lithium salt (9CI)
 MF C12 H14 O2 . Li



● Li

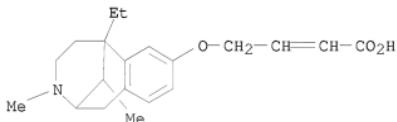
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 3-phenyl-4-(phenylthio)-, (Z)- (9CI)
 MF C16 H14 O2 S

Double bond geometry as shown.



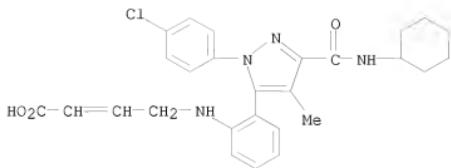
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(6-ethyl-1,2,3,4,5,6-hexahydro-3,11-dimethyl-2,6-methano-3-benzazocin-8-yl)oxy]-, sodium salt (9CI)
 MF C20 H27 N O3 . Na



● Na

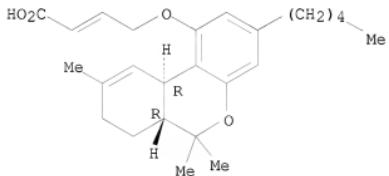
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(2-[1-(4-chlorophenyl)-3-[(cyclohexylamino)carbonyl]-4-methyl-1H-pyrazol-5-yl]phenyl]amino]-
 MF C27 H29 Cl N4 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

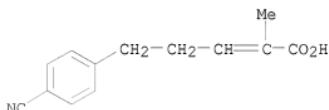
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(6aR,10aR)-6a,7,8,10a-tetrahydro-6,6,9-trimethyl-3-pentyl-6H-dibenzo[b,d]pyran-1-yl]oxy]-
 MF C25 H34 O4

Absolute stereochemistry.
 Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

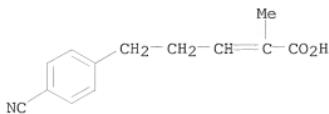
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Pentenoic acid, 5-(4-cyanophenyl)-2-methyl-
 MF C13 H13 N O2
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

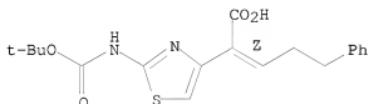
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Pentenoic acid, 5-(4-cyanophenyl)-2-methyl-, lithium salt (9CI)
MF C13 H13 N O2 . Li



● Li

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 4-Thiazaoleic acid, 2-[(1,1-dimethylethoxy)carbonyl]amino]- α -(3-phenylpropylidene)-, (Z)- (9CI)
MF C19 H22 N2 O4 S

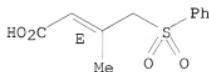
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

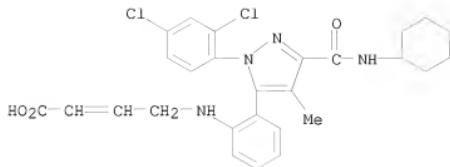
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 3-methyl-4-(phenylsulfonyl)-, (E)- (9CI)
MF C11 H12 O4 S

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[[2-[3-[(cyclohexylamino)carbonyll-1-(2,4-dichlorophenyl)-4-methyl-1H-pyrazol-5-yl]phenyl]amino]-
MF C27 H28 C12 N4 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

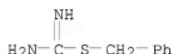
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-phenoxy-, (2E)-, compd. with phenylmethyl carbamimidothioate (1:1)
 MF C10 H10 O3 . C8 H10 N2 S

CM 1

Double bond geometry as shown.

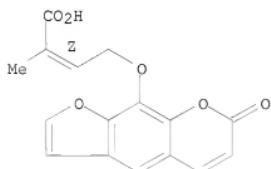


CM 2



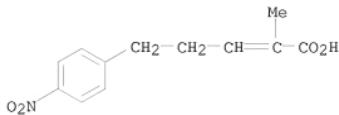
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 2-methyl-4-[(7-oxo-7H-furo[3,2-g][1]benzopyran-9-yl)oxy]-
 , (2Z)-
 MF C16 H12 O6

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

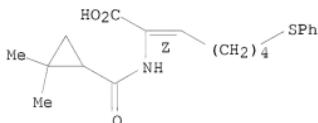
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Pentenoic acid, 2-methyl-5-(4-nitrophenyl)-, lithium salt (9CI)
MF C12 H13 N O4 . Li



● Li

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Heptenoic acid, 2-[(2,2-dimethylcyclopropyl)carbonyl]amino]-7-
(phenylthio)-, (Z)- (9CI)
MF C19 H25 N O3 S

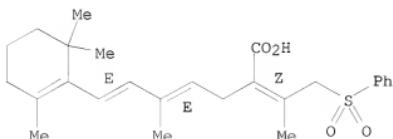
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

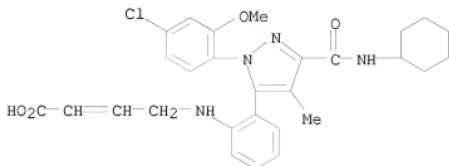
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 4,6-Heptadienoic acid, 5-methyl-2-[1-methyl-2-(phenylsulfonyl)ethylidene]-
7-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (Z,E,E)- (9CI)
MF C26 H34 O4 S

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

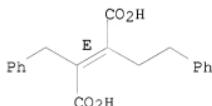
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(2-[1-(4-chloro-2-methoxyphenyl)-3-[(cyclohexylamino)carbonyl]-4-methyl-1H-pyrazol-5-yl]phenyl]amino]-
MF C28 H31 Cl N4 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

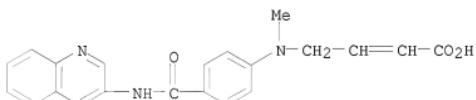
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenedioic acid, 2-(2-phenylethyl)-3-(phenylmethyl)-, (2E)-
MF C19 H18 O4

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

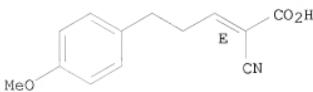
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[methyl[4-[(3-quinolinylamino)carbonyl]phenyl]amino]-
MF C21 H19 N3 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

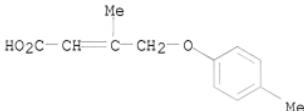
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Pentenoic acid, 2-cyano-5-(4-methoxyphenyl)-, (E)- (9CI)
MF C13 H13 N O3

Double bond geometry as shown.



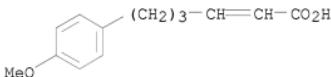
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Crotonic acid, 3-methyl-4-(p-tolyl)oxy- (7CI)
MF C12 H14 O3



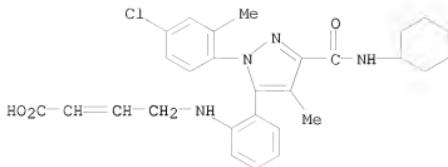
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Hexenoic acid, 6-(4-methoxyphenyl)-
MF C13 H16 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

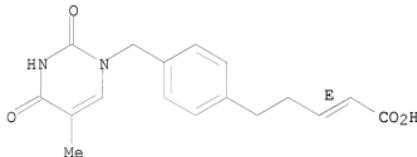
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(2-[(4-chloro-2-methylphenyl)-3-[(cyclohexylamino)carbonyl]-4-methyl-1H-pyrazol-5-yl]phenyl]amino)-
MF C28 H31 Cl N4 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

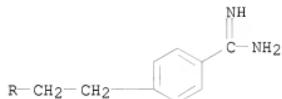
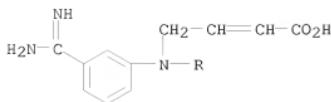
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Pentenoic acid, 5-[4-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)methyl]phenyl]-, (2E)-
 MF C17 H18 N2 O4

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

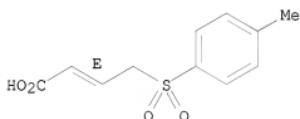
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(3-(aminociminomethyl)phenyl)[2-(4-(aminoiminomethyl)phenyl]ethyl]amino]-
 MF C20 H23 N5 O2
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(4-methylphenyl)sulfonyl]-, (E)- (9CI)
 MF C11 H12 O4 S

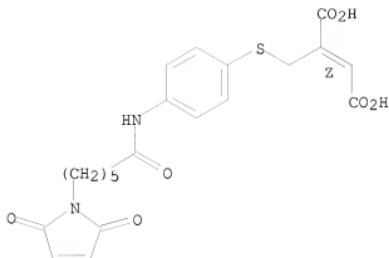
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenedioic acid, 2-[[[4-[(6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxohexyl)amino]phenyl]thio]methyl]-, (Z)- (9CI)
 MF C21 H22 N2 O7 S

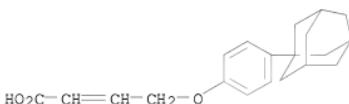
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

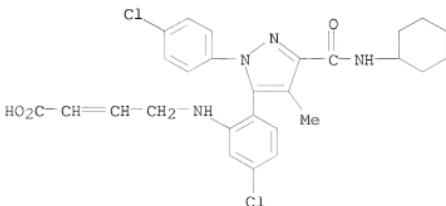
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-(4-tricyclo[3.3.1.13,7]dec-1-ylphenoxy)-
 MF C20 H24 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

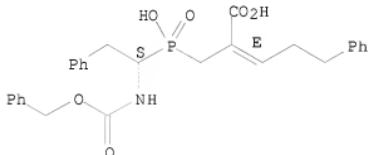
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(5-chloro-2-[1-(4-chlorophenyl)-3-
 [(cyclohexylamino)carbonyl]-4-methyl-1H-pyrazol-5-yl]phenyl]amino)-
 MF C27 H28 Cl2 N4 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

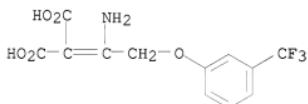
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Pentenoic acid, 2-[{hydroxy[(1*S*)-2-phenyl-1-
[(phenylmethoxy)carbonyl]amino]ethyl]phosphinyl]methyl]-5-phenyl-, (2E)-
MF C28 H30 N O6 P

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

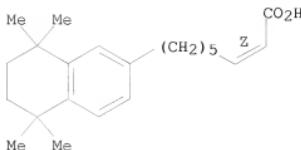
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Propanedioic acid, 2-[1-amino-2-[3-(trifluoromethyl)phenoxy]ethylidene]-
MF C12 H10 F3 N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

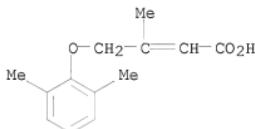
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Octenoic acid, 8-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-
, (Z)- (9CI)
MF C22 H32 O2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Crotonic acid, 3-methyl-4-(2,6-xylyloxy)- (7CI)
 MF C13 H16 O3

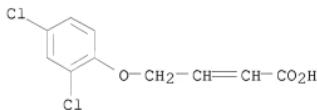


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-(2,4-dichlorophenoxy)-, compd. with N-methylmethanamine (1:1), mixt. with 3-(1-methylethyl)-1H-2,1,3-benzothiadiazin-4(3H)-one 2,2-dioxide compd. with N-methylmethanamine (1:1) (9CI)
 MF C10 H12 N2 O3 S . C10 H8 Cl2 O3 . C2 H7 N . C2 H7 N
 CI MXS

CM 1

CM 2

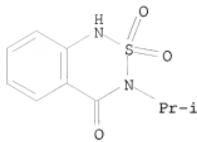


CM 3

H3C—NH—CH3

CM 4

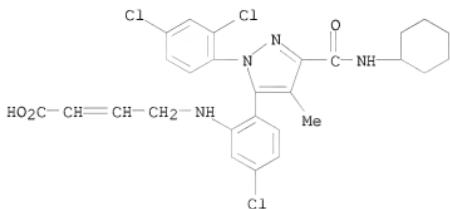
CM 5



CM 6

$$\text{H}_3\text{C}-\text{NH}-\text{CH}_3$$

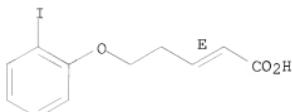
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[5-chloro-2-[3-[(cyclohexylamino)carbonyl]-1-(2,4-dichlorophenyl)-4-methyl-1H-pyrazol-5-yl]phenyl]amino]-
MF C27 H27 Cl3 N4 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

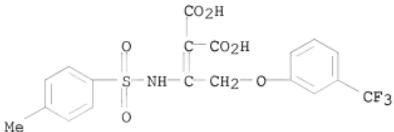
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Pentenoic acid, 5-(2-iodophenoxy)-, (2E)-
MF C11 H11 I O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

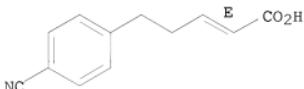
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Propanedioic acid, 2-[1-[(4-methylphenyl)sulfonyl]amino]-2-[3-(trifluoromethyl)phenoxy]ethylidene]-
MF C19 H16 F3 N O₇ S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Pentenoic acid, 5-(4-cyanophenyl)-, (E)- (9CI)
MF C12 H11 N O₂

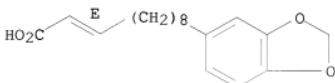
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Undecenoic acid, 11-(1,3-benzodioxol-5-yl)-, (E)- (9CI)
MF C18 H24 O₄

Double bond geometry as shown.

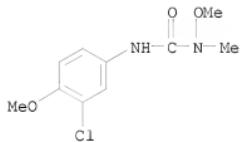


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-(2,4-dichlorophenoxy)-, compd. with N-methylmethanamine (1:1), mixt. with N'-(3-chloro-4-methoxyphenyl)-N-methoxy-N-methylurea

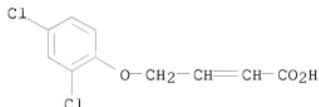
(9CI)
MF C10 H13 Cl N2 O3 . C10 H8 Cl2 O3 . C2 H7 N
CI MXS

CM 1



CM 2

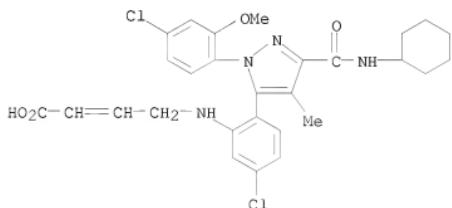
CM 3



CM 4

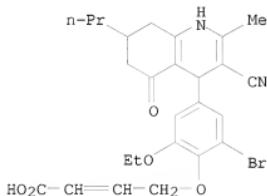
H3C-NH-CH3

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[5-chloro-2-[1-(4-chloro-2-methoxyphenyl)-3-[(cyclohexylamino)carbonyl]-4-methyl-1H-pyrazol-5-yl]phenyl]amino]-
MF C28 H30 Cl2 N4 O4



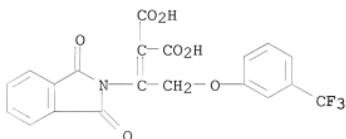
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[2-bromo-4-(3-cyano-1,4,5,6,7,8-hexahydro-2-methyl-5-oxo-7-propyl-4-quinolinyl)-6-ethoxyphenoxy]-
MF C26 H29 Br N2 O5



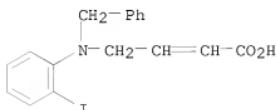
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Propanedioic acid, 2-[1-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-2-[3-(trifluoromethyl)phenoxy]ethylidene]-
MF C20 H12 F3 N O7



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

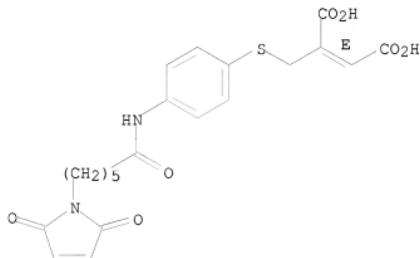
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(2-iodophenyl)(phenylmethyl)amino]-
MF C17 H16 I N O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

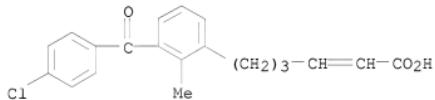
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenedioic acid, 2-[[4-[(6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxohexyl)amino]phenyl]thio]methyl]-, (E)- (9CI)
MF C21 H22 N2 O7 S

Double bond geometry as shown.



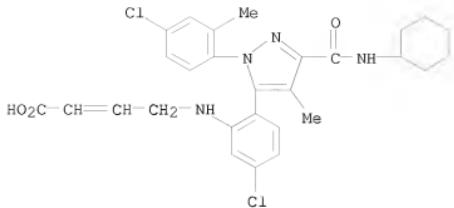
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Hexenoic acid, 6-[3-(4-chlorobenzoyl)-2-methylphenyl]-
MF C20 H19 Cl O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[[5-chloro-2-[1-(4-chloro-2-methylphenyl)-3-[(cyclohexylamino)carbonyl]-4-methyl-1H-pyrazol-5-yl]phenyl]amino]-
MF C28 H30 Cl2 N4 O3

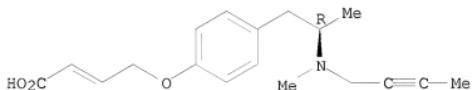


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

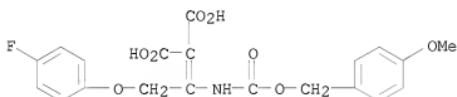
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[4-[(2R)-2-(2-butyn-1-ylmethylamino)propyl]phenoxy]-
 MF C18 H23 N O3

Absolute stereochemistry.
 Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

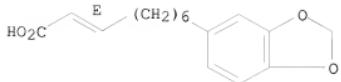
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Propanedioic acid, 2-[2-(4-fluorophenoxy)-1-[[[(4-methoxyphenyl)methoxy]carbonyl]amino]ethylidene]-
 MF C20 H18 F N O8



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

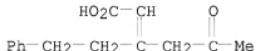
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Nonenenoic acid, 9-(1,3-benzodioxol-5-yl)-, (E)- (9CI)
 MF C16 H20 O4

Double bond geometry as shown.



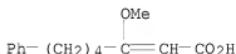
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Hexenoic acid, 5-oxo-3-phenethyl- (6CI)
MF C14 H16 O3



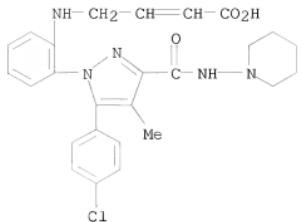
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Heptenoic acid, 3-methoxy-7-phenyl-
MF C14 H18 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

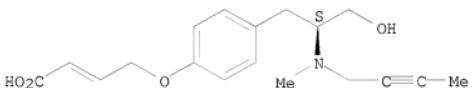
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(2-[5-(4-chlorophenyl)-4-methyl-3-[(1-piperidinylamino)carbonyl]-1H-pyrazol-1-yl]phenyl]amino]-
MF C26 H28 Cl N5 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

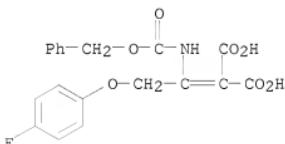
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[4-[(2S)-2-(2-butynylmethylamino)-3-hydroxypropyl]phenoxy]-
 MF C18 H23 N O4

Absolute stereochemistry.
 Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Propanedioic acid, 2-[2-(4-fluorophenoxy)-1-[(phenylmethoxy)carbonyl]aminooethylidene]-
 MF C19 H16 F N O7

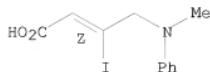


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 3-iodo-4-(methylphenylamino)-, (Z)- (9CI)

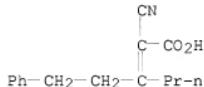
MF C11 H12 I N O2

Double bond geometry as shown.



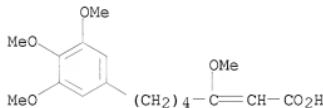
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Hexenoic acid, 2-cyano-3-phenethyl- (6CI)
MF C15 H17 N O2



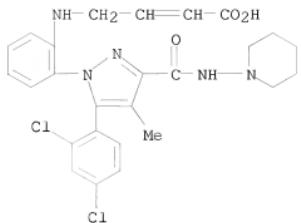
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Heptenoic acid, 3-methoxy-7-(3,4,5-trimethoxyphenyl)-
MF C17 H24 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

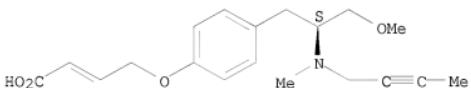
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(2-[5-(2,4-dichlorophenyl)-4-methyl-3-[(1-piperidinylamino)carbonyl]-1H-pyrazol-1-yl]phenyl]amino]-
MF C26 H27 Cl2 N5 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

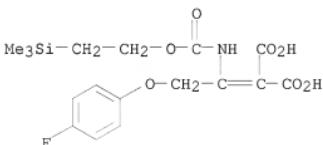
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[4-[(2S)-2-(2-butyn-1-ylmethylamino)-3-methoxypropylphenoxy]-
 MF C19 H25 N O4

Absolute stereochemistry.
 Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Propanedioic acid, 2-[2-(4-fluorophenoxy)-1-[(2-(trimethylsilyl)ethoxy]carbonyl]amino]ethylidene]-
 MF C17 H22 F N O7 Si



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Heptenoic acid, 7-phenyl-

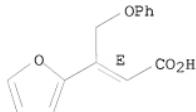
MF C13 H16 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 3-(2-furanyl)-4-phenoxy-, (E)- (9CI)
MF C14 H12 O4

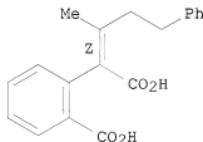
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

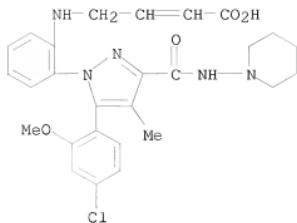
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Benzenesacetic acid, 2-carboxy- α -(1-methyl-3-phenylpropylidene)-,
(Z)- (9CI)
MF C19 H18 O4

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

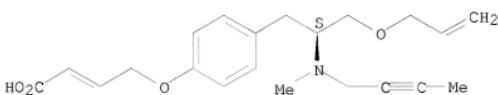
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(2-[5-(4-chloro-2-methoxyphenyl)-4-methyl-3-[(1-piperidinylamino)carbonyl]-1H-pyrazol-1-yl]phenyl]amino]-
MF C27 H30 Cl N5 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

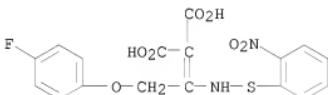
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[4-[(2S)-2-(2-butyn-1-ylmethylamino)-3-(2-propen-1-yloxy)propyl]phenoxy]-
MF C21 H27 N O4

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Propanedioic acid, 2-[2-(4-fluorophenoxy)-1-[(2-nitrophenyl)thio]amino]ethylidene]-
MF C17 H13 F N2 O7 S

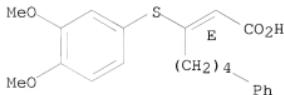


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Heptenoic acid, 3-[(3,4-dimethoxyphenyl)thio]-7-phenyl-, (E)- (9CI)
MF C21 H24 O4 S

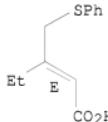
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Pentenoic acid, 3-[(phenylthio)methyl]-, (E)- (9CI)
MF C12 H14 O2 S

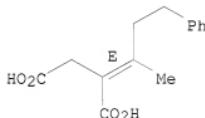
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

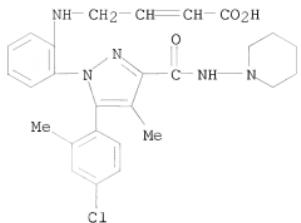
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Butanedioic acid, (1-methyl-3-phenylpropylidene)-, (E)- (9CI)
MF C14 H16 O4

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

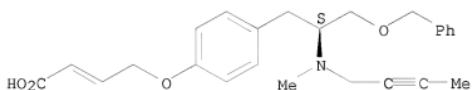
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(2-[(4-chloro-2-methylphenyl)-4-methyl-3-[(1-piperidinylamino)carbonyl]-1H-pyrazol-1-yl]phenyl]amino)-
MF C27 H30 Cl N5 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

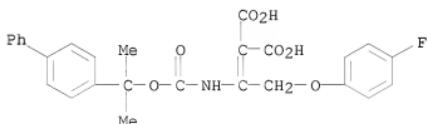
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[4-[(2S)-2-(2-butyn-1-ylmethylamino)-3-(phenylmethoxy)propyl]phenoxy]-
 MF C25 H29 N O4

Absolute stereochemistry.
 Double bond geometry unknown.



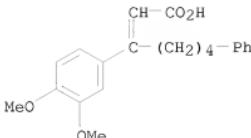
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Propanedioic acid, 2-[1-[(1-[1,1'-biphenyl]-4-yl-1-methylethoxy)carbonylamino]-2-(4-fluorophenoxy)ethylidene]-
 MF C27 H24 F N O7



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

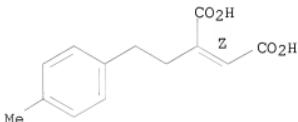
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Heptenoic acid, 3-(3,4-dimethoxyphenyl)-7-phenyl-
 MF C21 H24 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Maleic acid, (p-methylphenethyl)- (6CI)
 MF C13 H14 O4

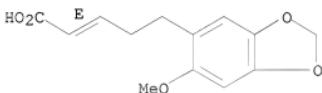
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

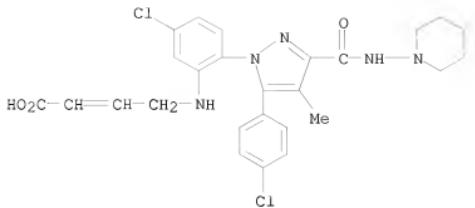
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Pentenoic acid, 5-(6-methoxy-1,3-benzodioxol-5-yl)-, (E)- (9CI)
 MF C13 H14 O5

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

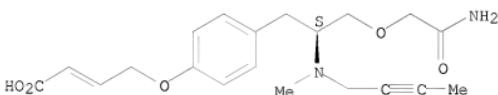
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[(5-chloro-2-[5-(4-chlorophenyl)-4-methyl-3-[(1-piperidinylamino)carbonyl]-1H-pyrazol-1-yl]phenyl]amino]-
 MF C26 H27 Cl2 N5 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

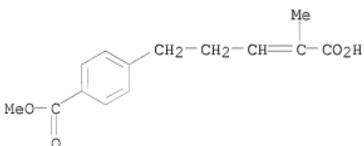
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[4-[(2S)-3-(2-amino-2-oxoethoxy)-2-(2-butyn-1-yl)methylamino]propyl]phenoxy]-
 MF C20 H26 N2 O5

Absolute stereochemistry.
 Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

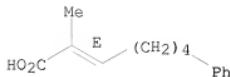
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Benzoic acid, 4-(4-carboxy-3-penten-1-yl)-, 1-methyl ester
 MF C14 H16 O4
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

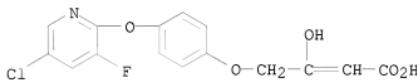
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Heptenoic acid, 2-methyl-7-phenyl-, (E)- (9CI)
 MF C14 H18 O2

Double bond geometry as shown.



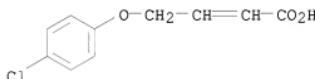
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[4-[(5-chloro-3-fluoro-2-pyridinyl)oxy]phenoxy]-3-
hydroxy-
MF C15 H11 Cl F N O5



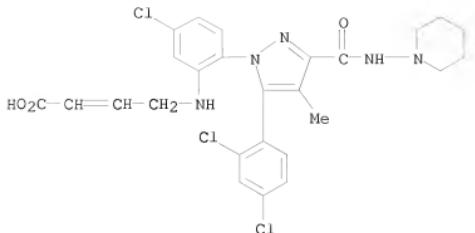
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-(4-chlorophenoxy)-, sodium salt (9CI)
MF C10 H9 Cl O3 . Na



● Na

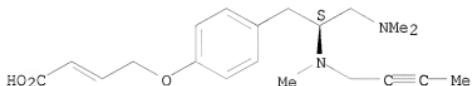
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[(5-chloro-2-[5-(2,4-dichlorophenyl)-4-methyl-3-[(1-
piperidinylamino)carbonyl]-1H-pyrazol-1-yl]phenyl]amino]-
MF C26 H26 Cl3 N5 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-[4-[(2S)-2-(2-butyn-1-ylmethylamino)-3-(dimethylamino)propyl]phenoxy]-
 MF C20 H28 N2 O3

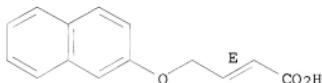
Absolute stereochemistry.
 Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-(2-naphthalenyloxy)-, (2E)-
 MF C14 H12 O3

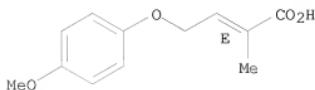
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

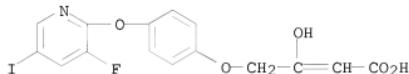
L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2-Butenoic acid, 4-(4-methoxyphenoxy)-2-methyl-, (E)- (9CI)
 MF C12 H14 O4

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 404 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Butenoic acid, 4-[4-[(3-fluoro-5-iodo-2-pyridinyl)oxy]phenoxy]-3-hydroxy-
MF C15 H11 F 1 N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> save temp l17 erset/a

ANSWER SET L17 HAS BEEN SAVED AS 'ERSET/A'

=> e 2-Hexenoic acid, 6-(4-methoxyphenyl)-/cn
E1 1 2-HEXENOIC ACID, 6-(4-HYDROXY-4-METHYL-2-OXOCYCLOHEXYL)-, ME
THYL ESTER, (1R-(1A(E),4A))-/-CN
E2 1 2-HEXENOIC ACID, 6-(4-HYDROXY-4-METHYL-2-OXOCYCLOHEXYL)-, ME
THYL ESTER, (1R-(1A(E),4B))-/-CN
E3 1 --> 2-HEXENOIC ACID, 6-(4-METHOXYPHENYL)-/-CN
E4 1 2-HEXENOIC ACID, 6-(4-METHOXYPHENYL)-, ETHYL ESTER/CN
E5 1 2-HEXENOIC ACID, 6-(4-METHOXYPHENYL)-, ETHYL ESTER, (2E)-/-CN
E6 1 2-HEXENOIC ACID, 6-(4-METHOXYPHENYL)-4,4-BIS(METHYLTHIO)-, E
THYL ESTER, (E)-/-CN
E7 1 2-HEXENOIC ACID, 6-(4-METHOXYPHENYL)-4-OXO-, ETHYL ESTER, (E
)-/-CN
E8 1 2-HEXENOIC ACID, 6-(4-METHOXYPHENYL)-6-OXO-, ETHYL ESTER, (2
E)-/-CN
E9 1 2-HEXENOIC ACID, 6-(4-METHYL-1-PIPERIDINYL)-5-((2-NAPHTHALEN
YLSULFONYL)AMINO)-6-OXO-, METHYL ESTER, (S)-/-CN
E10 1 2-HEXENOIC ACID, 6-(4-METHYL-2-OXO-3-CYCLOHEXEN-1-YL)-, METH
YL ESTER, (R-(E))-/-CN
E11 1 2-HEXENOIC ACID, 6-(4-METHYL-2-OXO-3-CYCLOHEXEN-1-YL)-, METH
YL ESTER, (R-(Z))-/-CN
E12 1 2-HEXENOIC ACID, 6-(4-METHYL-5-OXO-3-CYCLOHEXEN-1-YL)-, METH
YL ESTER, (E)-/-CN

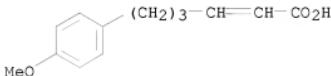
=> e3

L18 1 "2-HEXENOIC ACID, 6-(4-METHOXYPHENYL)-"/CN

=> d 118

L18 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

RN 52244-71-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Hexenoic acid, 6-(4-methoxyphenyl)- (CA INDEX NAME)
OTHER NAMES:
CN 6-(p-Methoxyphenyl)-2-hexenoic acid
MF C13 H16 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

| => file caplus | SINCE FILE | TOTAL |
|--|------------|---------|
| COST IN U.S. DOLLARS | ENTRY | SESSION |
| FULL ESTIMATED COST | 197.01 | 582.78 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| CA SUBSCRIBER PRICE | ENTRY | SESSION |
| | 0.00 | -1.60 |

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FILE COVERS 1907 - 19 Jun 2008 VOL 148 ISS 25
FILE LAST UPDATED: 18 Jun 2008 (20080618/ED)

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=> l18
L19 1 L18
=> d l19 ti fbib abs

L19 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

TI 1,5-Hydride shifts in acyclic systems containing α,β -unsaturated ketones and p-methoxyphenyl groups
 AN 1974:145604 CAPLUS
 DN 80:145604
 OREF 80:23497a,23500a
 TI 1,5-Hydride shifts in acyclic systems containing α,β -unsaturated ketones and p-methoxyphenyl groups
 AU Atkinson, Robert S.; Green, Richard H.
 CS Dep. Chem., Univ. Leicester, Leicester, UK
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1974), (3), 394-401
 CODEN: JCPRB4; ISSN: 0300-922X
 DT Journal
 LA English
 AB D-labeling showed that the acid-catalyzed rearrangement of p-HOC6H4(CH2)2CR2CH2CH:CHCOMe (I, R = H) to 2-(p-hydroxyphenyl)cyclohexyl Me ketone involved an intramol. H shift. A similar rearrangement was observed for I (R = Me) and its aromatic Me ether but not analogous products were obtained from p-MeOC6H4CHR(CH2)2CH:CHCOMe (R = H, p-MeOC6H4) under the same reaction conditions.

| | | | |
|--|------------------|---------------|--|
| => file reg | | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION | |
| FULL ESTIMATED COST | 5.31 | 588.09 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION | |
| CA SUBSCRIBER PRICE | -0.80 | -2.40 | |

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STRUCTURE FILE UPDATES: 18 JUN 2008 HIGHEST RN 1029146-45-9
 DICTIONARY FILE UPDATES: 18 JUN 2008 HIGHEST RN 1029146-45-9

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e 2-Heptenoic acid, 3-methoxy-7-phenyl-/cn
 E1 1 2-HEPTENOIC ACID, 3-METHOXY-7-(3,4-(METHYLENEDIOXY)PHENYL)-, METHYL ESTER/CN
 E2 1 2-HEPTENOIC ACID, 3-METHOXY-7-(4-METHOXYPHENYL)-6-OXO-, METHYL ESTER/CN
 E3 1 --> 2-HEPTENOIC ACID, 3-METHOXY-7-PHENYL-/CN

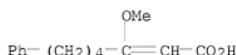
E4 1 2-HEPTENOIC ACID, 3-METHOXY-7-PHENYL-, (E)-/CN
 E5 1 2-HEPTENOIC ACID, 3-METHYL-/CN
 E6 1 2-HEPTENOIC ACID, 3-METHYL-, (2E)-/CN
 E7 1 2-HEPTENOIC ACID, 3-METHYL-, (2Z)-/CN
 E8 1 2-HEPTENOIC ACID, 3-METHYL-, (2Z)-, MIXT. WITH (3Z)-3-METHYL
 -3-HEPTENOIC ACID/CN
 E9 1 2-HEPTENOIC ACID, 3-METHYL-, (E)-/CN
 E10 1 2-HEPTENOIC ACID, 3-METHYL-, (E)-, COMPD. WITH N-CYCLOHEXYLC
 YCLOHEXANAMINE (1:1)/CN
 E11 1 2-HEPTENOIC ACID, 3-METHYL-, (E)-, MIXT. WITH 3-METHYLENEHEP
 TANOIC ACID, (E)-3-METHYL-3-HEPTENOIC ACID, (Z)-3-METHYL-2-H
 EPENOIC ACID AND (Z)-3-METHYL-3-HEPTENOIC ACID/CN
 E12 1 2-HEPTENOIC ACID, 3-METHYL-, (Z)-/CN

=> e3

L20 1 "2-HEPTENOIC ACID, 3-METHOXY-7-PHENYL-"/CN

=> d 120

L20 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
 RN 60427-87-4 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 2-Heptenoic acid, 3-methoxy-7-phenyl- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN α -Heptenoic acid, β -methoxy- ζ -phenyl- (3CI)
 MF C14 H18 O3
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

| | | | |
|--|------------|---------|--|
| => file caplus | | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL | |
| | ENTRY | SESSION | |
| FULL ESTIMATED COST | 7.61 | 595.70 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL | |
| | ENTRY | SESSION | |
| CA SUBSCRIBER PRICE | 0.00 | -2.40 | |

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=> l20
L21 3 L20

=> d 121 1-3 ti

L21 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
TI Synthesis of kavain, dihydrokavain, and analogs

L21 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
TI Constituents of kawa root. X. Kawain and dihydrokawain

L21 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
TI Constituents of the kawa root. VIII. Kawaiic acid

=> d 121 1-3 ti fbib abs

L21 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
TI Synthesis of kavain, dihydrokavain, and analogs
AN 1977:5263 CAPLUS
DN 86:5263
OREF 86:907a,910a
TI Synthesis of kavain, dihydrokavain, and analogs
AU Israeli, Z. H.; Smissman, E. E.
CS Sch. Pharm., Univ. Kansas, Lawrence, KS, USA
SO Journal of Organic Chemistry (1976), 41(26), 4070-4
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
GI



AB Kavain (I), dihydrokavain (II), and a number of new analogues of kava pyrones were prepared. Kavain and dihydrokavain were synthesized by a modification of the Reformatskii reaction in yields severalfold higher than described before. Several new analogues of the naturally occurring kava pyrones were synthesized in 10–60% yields by condensing the appropriate aldehyde with 4-methoxy-6-methyl-2-pyrene. The pyrones dehydrokavain and yangonin were obtained in much improved yields. Catalytic hydrogenation of pyrones gave new analogues of dihydrokavain.

L21 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
TI Constituents of kawa root. X. Kawain and dihydrokawain
AN 1931:8664 CAPLUS
DN 25:8664
OREF 25:937f-i,938a-b
TI Constituents of kawa root. X. Kawain and dihydrokawain
AU Borsche, W.; Peitzsch, W.
SO Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen
(1930), 63B, 2414-7
CODEN: BDCBAD; ISSN: 0365-9488
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C. A. 24, 1099-1100. It was shown in Paper VIII that kawaic acid (I) is the CH₂O₂-free mother substance of methysticin acid, CH₂O₂C₆H₃CH:CHC(OMe):CHCO₂H, and it was concluded that kawa root also probably contains, in addition to methysticin, C₁₅H₁₄O₅, the doubly unsatd. lactone kawain (II). Considerable difficulties were at first met in attempts to isolate it, but this was finally effected. Pure II is a beautifully crystallized substance, optically active like methysticin and extraordinarily similar to it in its chemical behavior. Hot NaOH smoothly converts it into I and catalytic hydrogenation gives a mixture of much dihydrokawain (III) and a little tetrahydrokawaic acid, PhCH₂CH₂CH₂CH₂CO₂(OMe):CHCO₂H (IV). III was also found (with J. Niemann) in kawa resin. Alkali isomerizes it to dihydrokawaic acid, PhCH₂CH₂CH:CHC(OMe):CHCO₂H (V). Com. kawa resin in 250-g. portions is dissolved in 2 l. Et₂O, filtered, the Et₂O shaken out 3 times with 3% NaOH, washed to neutrality with cold saturated NaCl, turbined several hrs. with Na₂SO₄ and evaporated, giving about 225 g. of residue. This is then extracted 10 hrs. daily for 6-7 days with petroleum-hexane in a continuous extractor, the extractive which seps. in the boiling flask being separately rinsed out every morning with Et₂O. When the combined Et₂O solns. are evaporated the residue begins to crystallize, especially if seeded with II and stirred. After several weeks the crystals are washed with Et₂O until the residue is colorless. Most of the II is present in the exts. of the 2nd-4th days and is obtained almost pure after 1 crystallization from MeOH-Et₂O. The total yield of II is about 25% of the purified resin. It is purified by distilling (195-7° under 0.1 mm.) and crystallizing from MeOH-Et₂O. It begins to sinter 102°, m. 105-6°, is soluble in concentrated H₂SO₄ with red color, [α]_D20 105° (1% solution in absolute alc.). III (3 g. from 4.6 g. II), m. 56-8°, soluble in H₂SO₄ without color, [α]_D20 30° (1% solution in absolute alc.). V, m. 139-40° (gas evolution). As III is more soluble than II, it is found in the Et₂O filtrates from the crude II obtained in the 2nd-4th day exts. of the resin. It seps. in yellowish crystalline aggregates, m. 50-4°, of a III-II mixture or "pseudokawain."

L21 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
TI Constituents of the kawa root. VIII. Kawaic acid
AN 1929:24992 CAPLUS
DN 23:24992
OREF 23:2965h-i,2966a-c
TI Constituents of the kawa root. VIII. Kawaic acid
AU Borsche, W.; Peitsch, W.
CS Univ. Frankfurt a. M.
SO Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen
(1929), 62B, 368-73
CODEN: BDCBAD; ISSN: 0365-9488
DT Journal
LA Unavailable

GI For diagram(s), see printed CA Issue.
AB The product C13H12O3, m. 164-5°, and designated as kawaic acid (I), which B. and Roth obtained from crude kawa resin, was not pure but admixed with nearly related acids, the separation of which has finally been effected only after many unsuccessful attempts. The pure I m. 185-6° and has the composition C14H24O3; it is evidently the CH202-free mother substance of methysticinic acid (II), i. e., γ -cinnamol- β -methoxycrotonic acid. Its Me ester on partial saponification with alc. HCl gives the same PhCH:CHCH:CHCOCH2CO2Me as is obtained by deacetylation of PhCH:CHCH:CHCOCHAcCO2Me. On catalytic reduction with colloidal Pd, I behaves just like II, taking up at first only 2 mols. H2 and giving tetrahydrokawaic acid (III), which on distillation in vacuo smoothly yields 6-phenyl-2-methoxy- Δ 1-hexene (IV), with acids is decomposed into MeOH, CO2 and 6-phenyl-2-hexanone and on further shaking with H2 and Pd is only very slowly reduced to hexahydrokawaic acid. III has been synthesized by treating PhCH2CH2CH2CH2COCH2CO2Me with a large excess of CH2N2 and saponifying the alkali-insol. part of the product with NaOH. A similar synthesis of I has not yet been effected because the double bonds in PhCH:-CHCH:CHCOCH2CO2Me react too easily with CH2N2 to form stable addition products containing N. I is obtained by B. and R.'s method from the kawa resin under exactly the same conditions as II from methysticin and it is, therefore, quite possible that I also does not exist in the resin as such but as a doubly unsatd. lactone, kawain, PhCH:-CHCH.CH2.C(OMe):CH.CO.O. I seps. from Et2O in yellow, elongated, 6-cornered tablets, soluble in concentrated H2SO4 with purple color, gives in MeOH with FeCl3 a faint brown color only after several hrs.; heated at 190° until the evolution of CO2 ceases, it yields a brown, glassy resin whose MeO content corresponds approx. to 6-phenyl-2-methoxy- Δ 1,3,6-hexatriene but which decomp. on attempted distillation under 14 mm. In N H2SO4 on the H2O bath I gives cinnamalacetone whose 2,4-dinitrophenylhydrazone, which can be obtained directly from I with HCl in boiling MeOH, brown-red, m. 218-20°. III, m. 109-10°, begins to evolve CO2 about 125°, gives no color in alc. with FeCl3. IV, refractive oil of faint odor, b18 136-8°.

=> 117/thu
275 L17
1019446 THU/RL
L22 21 L17/THU
(L17 (L) THU/RL)

=> d 122 1-21 ti

L22 ANSWER 1 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of maleic acid derivatives as metallo- β -lactamase inhibitors

L22 ANSWER 2 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Pyrazoles as cannabinoid receptor antagonists/inverse agonists useful for treating obesity

L22 ANSWER 3 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Metallo- β -lactamase inhibitors containing maleic acid derivatives, and use thereof with β -lactam antibiotics

L22 ANSWER 4 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI MAO-B inhibitors useful for treating obesity

L22 ANSWER 5 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI MAO-B inhibitors useful for treating obesity

L22 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Antitumoral activity of 13-demethyl or 13-substituted analogues of all-trans retinoic acid and 9-cis retinoic acid in the human myeloid leukemia cell line HL-60

L22 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Quinoline-derived amide modulators of vanilloid VR1 receptor, and their preparation, pharmaceutical compositions, and methods of use in the treatment of pain, inflammatory, and pulmonary conditions

L22 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of arylsulfonylpyranhydroxamates as matrix metalloprotease and/or aggrecanase inhibitors

L22 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of indole derivatives as phospholipase enzyme inhibitors for treatment of inflammatory conditions

L22 ANSWER 10 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of arylsulfonylpyranhydroxamates as matrix metalloprotease and/or aggrecanase inhibitors

L22 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of retinoic acid analogs for pharmaceutical use as retinoic acid receptor modulators

L22 ANSWER 12 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of diaryl carboxylic acids and derivatives as peroxisome proliferator-activated receptor ligands.

L22 ANSWER 13 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of arylsulfonates as follicle stimulating hormone antagonists.

L22 ANSWER 14 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of sulfonamides as pharmaceuticals with affinity for prostaglandin E2 receptors

L22 ANSWER 15 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of fused thiophene derivatives as interleukin-6 and interleukin-12 production inhibitors

L22 ANSWER 16 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of indole derivatives as phospholipase enzyme inhibitors

L22 ANSWER 17 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of phenylalkanoic acid derivatives as peroxisome proliferator-activated receptor controllers

L22 ANSWER 18 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of glutamic acid derivatives for the treatment of central nervous system disorders

L22 ANSWER 19 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of 3,5-bis(amidinophenyl)pentanoates and analogs as factor Xa inhibitors

L22 ANSWER 20 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
TI Topical preparations containing diphenylpyraline or other compounds for treatment of skin pigmentation

L22 ANSWER 21 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

substituent were prepared as leukotriene B₄ antagonists. Thus, amidation of 1,3-bis(carboxymethyl)-5-cinnamyl oxybenzene (I; R = R₁ = OH) (preparation given) with N-methyl-N-phenethylamine followed by esterification gave I (R = NMeCH₂CH₂Ph, R₁ = OMe), which was saponified to give leukotriene antagonist I (R = NMeCH₂CH₂Ph, R₁ = OH). Treatment of disorders which result from leukotriene B₄ activity using these monocyclic aryl compds. are disclosed.

| | | | |
|--|------------|---------|--|
| => logoff hold | | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL | |
| FULL ESTIMATED COST | ENTRY | SESSION | |
| | 29.60 | 625.30 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL | |
| CA SUBSCRIBER PRICE | ENTRY | SESSION | |
| | -3.20 | -5.60 | |

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 06:25:16 ON 19 JUN 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x::x

LOGINID:SSSPATA1623PAZ

PASSWORD:
* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 06:45:42 ON 19 JUN 2008
FILE 'CAPLUS' ENTERED AT 06:45:42 ON 19 JUN 2008
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| COST IN U.S. DOLLARS | SINCE FILE | TOTAL | |
| FULL ESTIMATED COST | ENTRY | SESSION | |
| | 29.60 | 625.30 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL | |
| CA SUBSCRIBER PRICE | ENTRY | SESSION | |
| | -3.20 | -5.60 | |

=> logoff hold

| | | | |
|--|------------|---------|--|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL | |
| FULL ESTIMATED COST | ENTRY | SESSION | |
| | 30.08 | 625.78 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL | |
| CA SUBSCRIBER PRICE | ENTRY | SESSION | |
| | -3.20 | -5.60 | |

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 06:46:01 ON 19 JUN 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x::x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

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FILE 'CAPLUS' ENTERED AT 07:45:32 ON 19 JUN 2008
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| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST | 30.08 | 625.78 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -3.20 | -5.60 |

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST | 30.56 | 626.26 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -3.20 | -5.60 |

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e 2-Butenoic acid, 2,3-dichloro-4-(methylphenylamino)-/cn
E1 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-(FORMYL METHYLAMINO)-4-OXO-,
(2Z)-/CN
E2 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-(METHYL(2-OXOETHYL)AMINO)-4-
OXO-, (2Z)-/CN
E3 1 --> 2-BUTENOIC ACID, 2,3-DICHLORO-4-(METHYLPHENYLAMINO)-/CN
E4 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-(METHYLPHENYLHYDRAZONO)-/CN
E5 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-(METHYLPHENYLHYDRAZONO)-, (Z
,?)-/CN
E6 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-(METHYLPHENYLHYDRAZONO)-, ME
THYL ESTER/CN
E7 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-(METHYLPHENYLHYDRAZONO)-, ME

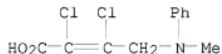
THYL ESTER, (Z,?)-/CN
 E8 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-(PHENYLHYDRAZONO)-/CN
 E9 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-(PHENYLHYDRAZONO)-, (Z,?)-/C
 N
 E10 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-(PHENYLHYDRAZONO)-, LABELED
 WITH CARBON-14, (Z,?)-/CN
 E11 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-(PHENYLIMINO)-, (2Z)-/CN
 E12 1 2-BUTENOIC ACID, 2,3-DICHLORO-4-OXO-/CN

=> e3

L23 1 "2-BUTENOIC ACID, 2,3-DICHLORO-4-(METHYLPHENYLAMINO)-"/CN

=> d 123

L23 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
 RN 623574-77-6 REGISTRY
 ED Entered STN: 04 Dec 2003
 CN 2-Butenoic acid, 2,3-dichloro-4-(methylphenylamino)- (CA INDEX
 NAME)
 MF C11 H11 Cl2 N O2
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

| | SINCE FILE
ENTRY | TOTAL
SESSION |
|--|---------------------|------------------|
| FULL ESTIMATED COST | 7.61 | 633.87 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE
ENTRY | TOTAL
SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -5.60 |

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=> l23
L24 1 L23

=> d l24 ti fbib abs

L24 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
TI Process for preparing highly functionalized γ -butyrolactams and
 γ -amino acids
AN 2003:892740 CAPLUS
DN 139:381742
TI Process for preparing highly functionalized γ -butyrolactams and
 γ -amino acids
IN Blazecka, Peter Garth; Davidson, James Guy, III; Zhang, Ji
PA Warner-Lambert Company LLC, USA
SO PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--|------|----------|-----------------|------------|
| PI | WO 2003093220 | A1 | 20031113 | WO 2003-IB1646 | 20030417 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
UG, US, UZ, VN, YU, ZA, ZM, ZW | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | US 2002-376991P | P 20020430 |
| US | 20030225149 | A1 | 20031204 | US 2003-365430 | 20030213 |
| | | | | US 2002-376991P | P 20020430 |
| CA | 2483830 | A1 | 20031113 | CA 2003-2483830 | 20030417 |
| | | | | US 2002-376991P | P 20020430 |
| | | | | WO 2003-IB1646 | W 20030417 |
| AU | 2003219425 | A1 | 20031117 | AU 2003-219425 | 20030417 |
| | | | | US 2002-376991P | P 20020430 |
| | | | | WO 2003-IB1646 | W 20030417 |
| EP | 1499583 | A1 | 20050126 | EP 2003-715236 | 20030417 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | US 2002-376991P | P 20020430 |
| | | | | WO 2003-IB1646 | W 20030417 |
| BR | 2003009743 | A | 20050209 | BR 2003-9743 | 20030417 |
| | | | | US 2002-376991P | P 20020430 |
| | | | | WO 2003-IB1646 | W 20030417 |
| CN | 1649827 | A | 20050803 | CN 2003-809641 | 20030417 |
| | | | | US 2002-376991P | P 20020430 |
| JP | 2005523932 | T | 20050811 | JP 2004-501360 | 20030417 |
| | | | | US 2002-376991P | P 20020430 |
| | | | | WO 2003-IB1646 | W 20030417 |
| US | 20030236415 | A1 | 20031225 | US 2003-421350 | 20030423 |

| | | | | |
|----------------|----|----------|-----------------|------------|
| US 6924377 | B2 | 20050802 | US 2002-376991P | P 20020430 |
| MX 2004PA10771 | A | 20050307 | MX 2004-PA10771 | 20041029 |
| | | | US 2002-376991P | P 20020430 |
| | | | WO 2003-IB1646 | W 20030417 |

OS CASREACT 139:381742; MARPAT 139:381742
 AB The invention relates to a process for preparing highly functionalized γ -butyrolactams and γ -amino acids by reductive amination of mucocholic acid or its derivs. and discloses a process for preparing pregabalin or 3-aminomethyl-5-methyloctanoic acid, GABA analogs with desirable medicinal activity. Claimed γ -amino acids have formula R1NHCH2CH(CHR2R3)CH2CO2H [R1 = alkyl, cycloalkyl, (CH2)0-3-aryl, -heterocyclyl, or -heteroaryl; R2, R3 = H, alkyl, alkenyl, cycloalkyl, alkylcycloalkyl, alkoxy, alkylphenyl, alkylphenoxy, or (un)substituted phenyl]. Thus, 1.3 g 5-(benzylxy)-4-isopropylidihydrofuran-2-one (prepared from mucochloric or mucobromic acid) was combined with 1.7 g ammonium formate, 0.3 g 20 % Pd/C, and 0.07 g [Ir(COD)Cl]2 in 25 mL MeOH. The mixture was hydrogenated at 70 °C and 20 psi for approx. 7 h to provide a mixture of pregabalin contaminated with 4-isopropylpyrrolidin-2-one. The mixture may be submitted to base hydrolysis to provide exclusively pregabalin.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
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 NEWS 8 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements
 NEWS 9 FEB 08 STN Express, Version 8.3, now available
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 NEWS 11 FEB 25 IFIREF reloaded with enhancements
 NEWS 12 FEB 25 IMSPRODUCT reloaded with enhancements
 NEWS 13 FEB 29 WPINDEX/WPIIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
 NEWS 14 MAR 31 IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats

| | | |
|---------|--------|---|
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| NEWS 16 | MAR 31 | CA/Caplus and CASREACT patent number format for U.S. applications updated |
| NEWS 17 | MAR 31 | LPCI now available as a replacement to LDPCI |
| NEWS 18 | MAR 31 | EMBASE, EMBAL, and LEMBASE reloaded with enhancements |
| NEWS 19 | APR 04 | STN AnaVist, Version 1, to be discontinued |
| NEWS 20 | APR 15 | WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats |
| NEWS 21 | APR 28 | EMBASE Controlled Term thesaurus enhanced |
| NEWS 22 | APR 28 | IMSRESEARCH reloaded with enhancements |
| NEWS 23 | MAY 30 | INPAFAMDB now available on STN for patent family searching |
| NEWS 24 | MAY 30 | DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option |
| NEWS 25 | JUN 06 | EPFULL enhanced with 260,000 English abstracts |
| NEWS 26 | JUN 06 | KOREPAT updated with 41,000 documents |
| NEWS 27 | JUN 13 | USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications |

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AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

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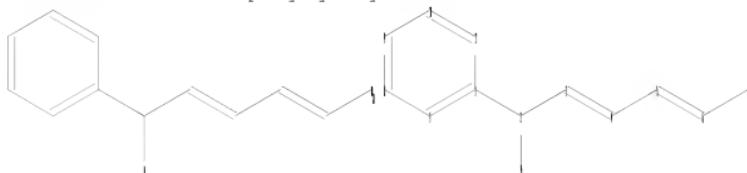
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10025947\10025947 phenylhydroxysorbic.str



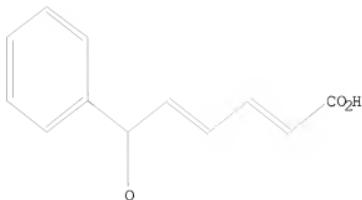
chain nodes :
2 3 4 5 6 14 15
ring nodes :
1 7 8 9 10 11
chain bonds :
1-2 2-3 2-15 3-4 4-5 5-6 6-14
ring bonds :
1-7 1-11 7-8 8-9 9-10 10-11
exact/norm bonds :
2-15
exact bonds :
1-2 2-3 3-4 4-5 5-6 6-14
normalized bonds :
1-7 1-11 7-8 8-9 9-10 10-11

G1:CH2,O,S,N

Hydrogen count :
2:>= minimum 1 3:>= minimum 1 4:>= minimum 1 5:>= minimum 1 6:>= minimum 1
Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 14:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR



G1 CH₂,O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam

SAMPLE SEARCH INITIATED 08:48:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 30 TO ITERATE

100.0% PROCESSED 30 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 272 TO 928
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> search l1 sss full

FULL SEARCH INITIATED 08:48:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 657 TO ITERATE

100.0% PROCESSED 657 ITERATIONS
SEARCH TIME: 00.00.01

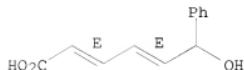
1 ANSWERS

L3 1 SEA SSS FUL L1

=> d scan

L3 1 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2,4-Hexadienoic acid, 6-hydroxy-6-phenyl-, (E,E)- (9CI)
MF C₁₂ H₁₂ O₃

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

```
=> file caplus
COST IN U.S. DOLLARS
SINCE FILE      TOTAL
ENTRY          SESSION
FULL ESTIMATED COST      178.82      179.03
```

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FILE COVERS 1907 - 19 Jun 2008 VOL 148 ISS 25
FILE LAST UPDATED: 18 Jun 2008 (20080618/ED)

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```
=> l3
L4      2 L3
```

```
=> d 14 1-2 ti fbib abs
```

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
TI Metabolites of the prototype insecticide (2E,4E)-N-isobutyl-6-phenylhexa-2,4-dienamide. 1. Synthesis, chromatography, spectroscopy, and biological activity
AN 1989:212302 CAPLUS
DN 110:212302
OREF 110:35219a,35222a
TI Metabolites of the prototype insecticide (2E,4E)-N-isobutyl-6-phenylhexa-2,4-dienamide. 1. Synthesis, chromatography, spectroscopy, and biological activity
AU Horsham, Mark A.; Class, Thomas J.; Johnston, John J.; Casida, John E.
CS Dep. Entomol. Sci., Univ. California, Berkeley, CA, 94720, USA
SO Journal of Agricultural and Food Chemistry (1989), 37(3), 777-81
CODEN: JAFCAU; ISSN: 0021-8561
DT Journal
LA English
AB Ten candidate metabolites of the prototype insecticide (2E,4E)-N-isobutyl-6-phenylhexa-2,4-dienamide (I) are prepared via a hydrozirconation procedure for stereospecific formation of the (2E,4E)-diene unit. This involves coupling vinylzirconocenes (derived from appropriately protected terminal acetylenes and dicyclopentadienylzirconium chloride hydride with vinyl halides under palladium(0) catalysis in 38-57% yield. Standard deprotection and functionalization methodol. yield the β -hydroxyisobutyl, 6-hydroxy, 6-keto, and p-hydroxy derivs. of I, the resp. carboxylic acid and amide and their 1-hydroxy derivs., and the β -hydroxyisobutyl, 6-hydroxy

derivative of I. The hydroxamic acid is prepared by condensing ,O-bis(trimethylsilyl)hydroxylamine with the acid chloride followed by hydrolysis. HPLC and GC-MS readily distinguish I and its derivs. (or their methylation products) for metabolite anal. Each of the candidate metabolites synthesized is less than one-third as toxic as I to piperonyl butoxide pretreated houseflies by injection and to mice by i.p. administration.

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
TI Metabolites of the prototype insecticide (2E,4E)-N-isobutyl-6-phenylhexa-2,4-dienamide. 2. Formation in mouse and rat liver microsomal systems, rat hepatocytes, and houseflies
AN 1989:207488 CAPLUS
DN 110:207488
OREF 110:34327a,34330a
TI Metabolites of the prototype insecticide (2E,4E)-N-isobutyl-6-phenylhexa-2,4-dienamide. 2. Formation in mouse and rat liver microsomal systems, rat hepatocytes, and houseflies
AU Johnston, John J.; Horsham, Mark A.; Class, Thomas J.; Casida, John E.
CS Dep. Entomol. Sci., Univ. California, Berkeley, CA, 94720, USA
SO Journal of Agricultural and Food Chemistry (1989), 37(3), 781-6
CODEN: JAFCAU; ISSN: 0021-8561
DT Journal
LA English
AB The metabolism of (2E,4E)-N-isobutyl-6-phenylhexa-2,4-dienamide is examined as
a prototype of the natural and synthetic isobutylamide insecticides. Nine metabolites from mouse and rat liver microsomal systems, rat hepatocytes, and/or houseflies are identified by HPLC, GC, and GC-mass spectrometric comparisons with synthetic stds. The parent isobutylamide yields the corresponding unsubstituted amide and N-methylene hydroxylation in the microsomal oxygenase system. Both of these amides are readily hydrolyzed by rat but not mouse amidases. The unsubstituted amide in mouse microsomes appears to undergo sequential enzymic oxidation and hydrolysis to the corresponding carboxylic acid; the presumed hydroxamic acid intermediate is not detected. Addnl. metabolites are the β -hydroxyisobutyl, 6-hydroxy, 6-keto, and p-hydroxy derivs. of the parent isobutylamide and the 6-hydroxy derivs. of the N-(β -hydroxyisobutyl) compound and of the unsubstituted amide and carboxylic acid. Hepatocytes conjugate some of these metabolites. The persistence and toxicity of this prototype insecticide are limited by oxidative metabolism at multiple sites in the iso-Bu and benzyl moieties.

=> logoff hold
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 8.22 187.25

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE -1.60 -1.60

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